# On Minimizers of

# Causal Variational Principles


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## Abstract

Causal variational principles are a class of nonlinear minimization problems which arise in a formulation of relativistic quantum theory referred to as the fermionic projector approach. This thesis is devoted to a numerical and analytic study of the minimizers of a general class of causal variational principles.

We begin with a numerical investigation of variational principles for the fermionic projector in discrete space-time. It is shown that for sufficiently many space-time points, the minimizing fermionic projector induces non-trivial causal relations on the space-time points. We then generalize the setting by introducing a class of causal variational principles for measures on a compact manifold. In our main result we prove under general assumptions that the support of a minimizing measure is either completely timelike, or it is singular in the sense that its interior is empty. In the examples of the circle, the sphere and certain flag manifolds, the general results are supplemented by a more detailed analysis of the minimizers.



## Zusammenfassung

Kausale Variationsprinzipien beschreiben eine Klasse nichtlinearer Minimierungsprobleme, die bei der Formulierung relativistischer Quantentheorie mittels des sogenannten fermionischen Projektors verwendet werden. Die vorliegende Dissertation widmet sich numerischen und analytischen Untersuchungen einer allgemeinen Klasse von kausalen Variationsprinzipien.

Numerische Untersuchungen von Variationsprinzipien auf fermionischen Projektoren zeigen, dass bei einer hinreichend großen Anzahl von Raumzeitpunkten der minimierende fermionische Projektor nichttriviale kausale Relationen auf den Raumzeitpunkten induziert. Als Verallgemeinerung wird eine Klasse von kausalen Variationsprinzipien für Maße auf einer kompakten Mannigfaltigkeit eingeführt. Das Hauptresultat zeigt, dass der Träger eines minimierenden Maßes entweder generisch zeitartig ist oder singulär ist in dem Sinne, dass das Innere des Trägers leer ist. Die allgemeinen Resultate werden ergänzt durch eingehende Untersuchungen der Minimierer von Beispielen auf dem Kreis, auf der Sphäre und auf bestimmten Fahnenmannigfaltigkeiten.

# Contents

# 1 Introduction

In the last century, experiments showed that classical Newtonian physics was not sufficient to explain effects which appeared either on cosmologically large or atomically small length scales. Thus the physical conception had to be changed and expanded with two new theories: the theory of general relativity and quantum theory. These theories only work on particular scales. By now one can not explain all quantum effects in the presence of gravity. At present, much research has been done to handle this dichotomy (i.e. [9]), but until now, the theories appear to be too contrary for a unification. The most renowned approaches for a formulation of quantum gravity are String Theory and Loop Quantum Gravity.

One approach in [9] to formulate relativistic quantum theory is "the principle of the fermionic projector", which was introduced in [10]. In this approach, the underlying space is assumed to be discrete on the Planck scale, where on the ensemble of discrete points a finite number of wave functions acts. The interaction of the particles is described by an action principle, whose minimizer shall contain all physical informations on the system. Additional structures, like non-trivial relations between the discrete space-time points and discrete causality, generate spontaneously. In a suitable limit (see [14]), the discrete causal space-time should go over to the causal structure of a Lorentzian manifold and the fermionic projector to a projector onto the Dirac sea of negative energy states.

The considerations of causal variational principles presented in this thesis are based on the following studies: In [12] it has been shown that the variational principle on fermionic projectors in discrete space-time is well-defined. A spontaneous breaking of the permutation symmetry of the space-time points has been discussed in [11], which has been further illustrated for small systems in [5]. These principles were introduced in [15] in a broader mathematical context as causal variational principles on measure spaces, where general existence results have been shown and examples have been discussed. In this thesis, we will try to deepen the understanding of causal variational principles and investigate in examples the emergence of additional structures, which will be both physically important and mathematically remarkable.

We will now present a structural overview and point out the main results: In Chapter 2, we introduce the variational principle in both space-time and particle representation and show the transition between the two approaches. In particle representation, the variational problem is given as a matrix problem: For matrices $F_x$, which sum to identity and have at most one positive, one negative simple eigenvalue, the Lagrangian is defined via the eigenvalues $\lambda_+$ and $\lambda_-$ of $F_x F_y$ as

$$\mathcal{L}[F_x, F_y] = \max\left(\tfrac{1}{2}\left(\lambda_+ - \lambda_-\right)^2, 0\right).$$

The variational principle minimizes the sum of the Lagrangians of all space-time points. The discrete causal structure on the space-time is introduced via the sign of the argument function $\mathcal{D}[F_x, F_y] = \frac{1}{2}(\lambda_+ - \lambda_-)^2$ of the Lagrangian $\mathcal{L}$.

If the eigenvalues of the matrices $F_x$ all coincide, the family of matrices can be identified with vectors on the two-sphere in the case of two particles, or in general with elements in a certain flag manifold. This is discussed in Chapter 3. The variational principle on fermionic projectors is analyzed for small systems analytically and numerically in Chapter 4. In addition to the already discussed symmetry breaking, a non-trivial causal structure appears.

In order to achieve a deeper understanding, we investigate the problem restricted to the family $\mathcal{F}$ of matrices $F_x$ with two prescribed eigenvalues. In Chapter 5, we study the variational principle in the case of two particles, which can be reformulated as a minimization problem on the sphere. Numerical studies show the occurrence of two interesting effects: For a sufficiently large number, points on the sphere coincide. Interpreting the number of points occupying the cluster point as weighting factor, the variational principle can consequently be understood as a variational principle on measures. The numerical outcomes show that the minimizing measure is supported only on a finite number of points. Thus the variational principle spontaneously generates a discrete structure on the sphere, an effect which can be interpreted as "quantization". Additionally, the structure of the minimizer changes, there emerges a "phase transition" between minimizers where all points in the support are timelike separated, and minimizers supported at only a finite number of points.

Motivated by these findings, in Chapter 6 we introduce causal variational principles in a general context: For a compact manifold $\mathcal{F}$, let $\mathcal{D}$ be a smooth real-valued function on $\mathcal{F} \times \mathcal{F}$. Defining the Lagrangian as $\mathcal{L} = \max(0, \mathcal{D})$, the causal variational principle is given by

$$\min_{\rho} \iint_{\mathcal{F}\times\mathcal{F}} \mathcal{L}(x,y)\, d\rho(x)\, d\rho(y),$$

where $\rho$ is a Borel measure on $\mathcal{F}$. We prove under general assumptions that the minimizers are either generically timelike (see Definition 6.11) or the support of the minimizing measure $\rho$ is singular in the sense that its interior is empty (see Theorem 6.19 and Theorem 6.21). In Chapter 7, we apply these general results to our model examples. Restricting the variational principle to the circle, we prove the phase transition and construct many minimizers in closed form. Again considering the variational principle on the sphere, we prove using the general results the phase transition and estimate the action from above and below.

In Chapter 8, we finally consider causal variational principles on the family of hermitian matrices with two prescribed eigenvalues of arbitrary dimension. After declaring the invariant measure and calculating the volume of the light-cones, we adapt our general results and prove that minimizers with singular support exist. Concluding, we estimate the action from above and conjecture the phase transition.

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# 2 Introduction of Causal Variational Principles on Fermion Systems

## 2.1 The Causal Variational Principle in Discrete Space-Time

We begin introducing the foundational structures in the space-time representation, see [12] and [5]. For an introduction and supplementary details on indefinite inner product spaces, see [1] and [17].

For $m \in \mathbb{N}$ let $H$ be a $2m$-dimensional complex vector space endowed with an *inner product* $\langle .|. \rangle$, that is a Hermitian sesquilinear form $\langle .|. \rangle : H \times H \to \mathbb{C}$. The inner product is supposed to be indefinite, thus there exist vectors which are *positive, negative* or *neutral*, i.e.

$$x \in H \text{ with } \langle x|x \rangle > 0, < 0 \text{ or } = 0.$$

A subspace $U \subset H$ is called *positive definite/negative definite* if all non-zero vectors in $U$ are positive/negative. We assume that the inner product is *non-degenerate*, which means that if $\langle u|v \rangle = 0$ for all $v \in H$ then it is $u = 0$, and that it has signature $(m, m)$. In this case, the space $H$ admits an orthogonal decomposition

$$H = H^+ \oplus H^-,$$

where $H^\pm$ are $m$-dimensional positive definite/negative definite subspaces.

The terminology of operators acting on Hilbert spaces can be transferred to indefinite inner product spaces: Let $A : H \to H$ be a linear operator acting on $H$. The *adjoint* of $A$ is the unique linear operator $A^* : H \to H$ that satisfies the equation

$$\langle Au|v \rangle = \langle u|A^* v \rangle \quad \text{for all} \quad u, v \in H.$$

The operator $A$ is called *self-adjoint* if $A^* = A$, and *unitary* if $A^* = A^{-1}$. The operator $A$ is a *projector* if it is self-adjoint and idempotent, $A = A^* = A^2$.

**Definition 2.1.** *Let $(E_x)_{x \in M}$ be a family of projectors on $H$ associated to the finite set $M = \{1, \ldots, m\}$. The projectors $(E_x)_{x \in M}$ are called* ***space-time projectors*** *if*

*i) the family is complete and orthogonal*

$$\sum_{x \in M} E_x = \mathbb{1} \quad \textit{and} \quad E_x \, E_y = \delta_{xy} \, E_x \quad \textit{for all} \quad x, y \in M, \tag{2.1.1}$$

*ii) for all $x \in M$ the inner product space $E_x(H)$ is non-degenerate and has signature $(1,1)$.*

*The set $(H, \langle .|. \rangle, (E_x)_{x \in M})$ is called* ***discrete space-time of spin dimension one****. An element $x \in M$ is referred to as* ***discrete space-time point****, where $m$ is the number of space-time points.*

We remark that for a generalization to arbitrary spin dimension $n$ it is demanded that the subspaces $E_x(H)$ have signature $(n,n)$, where $H$ has signature $(mn, mn)$. The fundamental object is introduced in the following Definition:

**Definition 2.2.** *A* ***fermionic projector*** *is a projector $P$ on $H$ whose image $P(H)$ is a negative definite subspace of $H$. The rank $f$ of $P$ is called* ***number of particles****. The set $(H, \langle .|. \rangle, (E_x)_{x \in M}, P)$ is called* ***fermion system in discrete space-time*** *or in short* ***discrete fermion system****.*

Since the image of $P$ is a subset of the maximal negative definite subspace of $H$, the number of particles is bounded by

$$1 \leq f \leq m. \tag{2.1.2}$$

The space-time projectors decompose the space $H$ into mutually orthogonal subspaces,

$$H = \bigoplus_{x \in M} E_x(H) \;,$$

and can be used to restrict operators to space-time points:

**Definition 2.3.** *The* ***discrete kernel*** *$P(x,y)$ is the localization of the fermionic projector $P$ at space-time points $x, y \in M$, regarded as a mapping restricted to the subspaces,*

$$P(x,y) = E_x \, P \, E_y : E_y(H) \longrightarrow E_x(H). \tag{2.1.3}$$

*The* ***closed chain*** *$A_{xy}$ is defined by*

$$A_{xy} = P(x,y) \, P(y,x) : E_x(H) \longrightarrow E_x(H). \tag{2.1.4}$$

The trace of the discrete kernel $P(x,x)$ is called *local trace* of $P$ at the space-time point $x$. According to the completeness of the space-time projectors (2.1.1), the local traces fulfill the relation

$$\sum_{x \in M} \mathrm{Tr}(P(x,x)) = \mathrm{Tr}(P) = f. \tag{2.1.5}$$

The closed chain $A_{xy}$ is a self-adjoint endomorphism acting on the two-dimensional inner product space $E_x(H)$. We define the action of a fermionic projector in terms of the eigenvalues of the closed chains:

**Definition 2.4.** *Let $\lambda_+$ and $\lambda_-$ denote the (complex) eigenvalues of the endomorphism $A_{xy}$ acting on $E_x(H)$, counted with algebraic multiplicities. Then the* ***spectral weight*** *of $A_{xy}$ is defined as*

$$|A_{xy}| = |\lambda_+| + |\lambda_-|\,.$$

*The* ***Lagrangian*** *of the closed chain $A_{xy}$ is given by*

$$\mathcal{L}[A_{xy}] = |A_{xy}^2| - \frac{1}{2}\,|A_{xy}|^2\,. \tag{2.1.6}$$

*Summing over all space-time points yields the* ***action*** *of the fermionic projector*

$$\mathcal{S}[P] = \sum_{x,y \in M} \mathcal{L}[A_{xy}]. \tag{2.1.7}$$

The variational principle is

$$\boxed{\textbf{minimize } \mathcal{S}[P] \textbf{ by varying } P} \tag{2.1.8}$$

keeping the discrete space-time and the number of particles $f$ fixed.

A simple computation shows the following representation of the Lagrangian:

**Corollary 2.5.** *If $\lambda_\pm$ denote the eigenvalues of $A_{xy}$, the Lagrangian can be written as*

$$\mathcal{L}[A_{xy}] = \frac{1}{2}\Big(|\lambda_+| - |\lambda_-|\Big)^2. \tag{2.1.9}$$

This transformations shows that the Lagrangian is a non-negative function, and consequently the action is bounded from below. The variational principle will try to achieve that the eigenvalues of all closed chains have nearly the same absolute value, in which case the Lagrangian gets small or even vanishes.

Assuming an additional technical condition, the minimum in (2.1.8) is attained:

**Theorem 2.6.** *Assume $(P_k)$ is a minimal sequence of (2.1.8) whose local trace is bounded away from zero in the sense that for a suitable $\delta > 0$*

$$|\mathrm{Tr}(E_x P_k)| > \delta \quad \textit{for all} \quad x \in M,\ k \in \mathbb{N}.$$

*Then there exists a minimizer $P$.*

For the proof, we refer to [12, Theorem 2.3]. The minimal action will be denoted by $\mathcal{S}_{\min}$. The parameters $f$ and $m$ affect the minimal action. Increasing the number of space-time points, the minimal action decreases, as shown in [12, Chapter 5]:

**Proposition 2.7.** *Let $\mathcal{S}_{\min}(m)$ denote the minimal action of a discrete space-time of $m$ space-time points with $f$ particles. Then the minimal action of a space-time of $m+1$ space-time points and $f$ particles can be estimated as*

$$\mathcal{S}_{\min}(m+1) \leq \left(1 - \frac{3}{4m}\right) \mathcal{S}_{\min}(m). \tag{2.1.10}$$

We now enlarge on the properties of the induced objects. Relative to a basis of $H$, the inner product $\langle .|. \rangle$ is represented by a Hermitian matrix $S \in \text{Mat}(2m \times 2m, \mathbb{C})$ such that

$$\langle u|v \rangle = (u|Sv) \quad \text{for all} \quad u, v \in H,$$

where $(.|.)$ denotes the standard Euclidean scalar product on $\mathbb{C}^{2m}$ . The non-degeneracy of the inner product is equivalent to $S$ being invertible, and the signature of $H$ coincides with the number of positive and negative eigenvalues of $S$, respectively. By choosing a suitable basis of $H$, the matrix $S$ can be written as signature matrix, i.e. a diagonal matrix with diagonal entries $\pm 1$. In view of the space-time decomposition, we can choose a basis such that the signature matrix $S$ on $H$ is represented in block matrix notation by

$$S = \begin{pmatrix} s & & \\ & \ddots & \\ & & s \end{pmatrix} \quad \text{for} \quad s = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2.1.11}$$

and the space-time projectors by

$$E_1 = \begin{pmatrix} \mathbb{1}_2 & & & \\ & 0 & & \\ & & \ddots & \\ & & & 0 \end{pmatrix} \quad , \quad \ldots \quad , \quad E_m = \begin{pmatrix} 0 & & & \\ & \ddots & & \\ & & 0 & \\ & & & \mathbb{1}_2 \end{pmatrix}. \tag{2.1.12}$$

In this basis, the adjoint of a linear operator $A$ on $H$ is represented by

$$A^* = SA^\dagger S, \tag{2.1.13}$$

where $^\dagger$ denotes the hermitian conjugate matrix. The self-adjointness of $P$ yields that the discrete kernels satisfy the relations

$$P(y,x) = P(x,y)^* = s\, P(x,y)^\dagger\, s \quad \text{for all} \quad x, y \in M.$$

The matrix $s$ is the signature matrix of the inner product restricted to $E_x(H)$. We next state an elementary relation, and refer to [19, Theorem 1.3.20] for the proof.

**Proposition 2.8.** *Let $A \in \text{Mat}(n \times m, \mathbb{C})$, $B \in \text{Mat}(m \times n, \mathbb{C})$ with $m \leq n$. Then the non-trivial eigenvalues of $AB$ and $BA$ counted with multiplicities coincide, and the characteristic polynomials of $AB$ and $BA$ satisfy the relation*

$$\det(AB - \lambda \mathbb{1}_n) = \lambda^{n-m} \det(BA - \lambda \mathbb{1}_m). \tag{2.1.14}$$

With regard to this relation, we conclude that the spectral weight and thus the Lagrangian is symmetric in its arguments,

$$\mathcal{L}[A_{xy}] = \mathcal{L}[A_{yx}] \quad \text{for all} \quad x, y \in M.$$

Using Proposition 2.8, we can prove the spectral theorem for self-adjoint operators on inner product spaces, [17, Chapter 4.2]:

**Proposition 2.9.** *Let $(H, \langle .|. \rangle)$ be a non-degenerate inner product space, and $A$ be a linear self-adjoint operator on $H$. Then the spectrum of $A$ lies symmetric relative to the real axis.*

*Proof.* Let $S$ denote the signature matrix of $\langle .|. \rangle$. Then using the commutation law (2.1.14) and formula (2.1.13) for the adjoint, it is

$$\overline{\det(A - \lambda \mathbb{1})} = \det(A^\dagger - \overline{\lambda} \mathbb{1}) = \det(S A^\dagger S - \overline{\lambda} \mathbb{1}) = \det(A^* - \overline{\lambda} \mathbb{1}),$$

which gives the claim. □

Consequently, the two non-trivial eigenvalues of the closed chain $A_{xy}$ are either both real or else build a complex conjugate pair. This spectral property offers the introduction of a notion of causality in discrete space-time, compare [29]:

**Definition 2.10** (causal structure). *Two space-time points $x, y \in M$ are called*

$$\begin{cases} \textbf{\textit{spacelike separated}} \text{ if the eigenvalues of } A_{xy} \text{ lie in } \mathbb{C} \backslash \mathbb{R}, \\ \textbf{\textit{timelike separated}} \text{ if the eigenvalues of } A_{xy} \text{ are real and non-zero}, \\ \textbf{\textit{lightlike separated}} \text{ if the eigenvalues of } A_{xy} \text{ vanish}. \end{cases}$$

*We define the sets*

$$\begin{aligned} \mathcal{I}(x) &= \{ y \text{ timelike separated from } x \} && \text{open light-cone} \\ \mathcal{J}(x) &= \{ y \text{ non-spacelike separated from } x \} && \text{closed light-cone} \\ \mathcal{K}(x) &= \{ y \text{ lightlike separated from } x \} && \text{boundary of the light-cone}. \end{aligned}$$

According to Proposition 2.8, the notion of causality is symmetric in $x, y$. Spacelike or lightlike separated points do not contribute to the action since the Lagrangian $\mathcal{L}[A_{xy}]$ in these cases vanishes.

We next discuss the symmetries of the setting, see [11]. Let $\mathrm{U}(H)$ denote the set of linear operators acting on $H$ which are unitary with respect to the inner product $\langle .|. \rangle$. A unitary transformation of the whole system does not change the action, but changes the structure of the system.

**Definition 2.11.** *A unitary transformation of the fermionic projector $P$ by an operator $U \in \mathrm{U}(H)$*

$$P \to UPU^*$$

*which does not change the space-time, i.e.*

$$U\, E_x\, U^* \;=\; E_x \quad \text{for all} \quad x \in M,$$

*is called* ***gauge transformation****. The group of gauge transformations is denoted by* $\mathcal{G}$*. If the fermionic projector remains unchanged,* $UPU^* = P$*, the operator* $U \in \mathcal{G}$ *is called* ***gauge symmetry****.*

Gauge transformations are *inner symmetries* since they only act locally on the spaces $E_x(H)$ but keep the discrete space-time unchanged. The gauge group splits up into a direct sum of unitary transformations $U_x := E_x U E_x \in \mathrm{U}(E_x(H)) \simeq \mathrm{U}(1,1)$ which act unitarily on $E_x(H)$.

A transformation that also permutes the space-time points will be called *outer symmetry*. Let $S_m$ denote the symmetric group on $M$:

**Definition 2.12.** *A subgroup* $\mathcal{O} \subset S_m$ *is called* ***outer symmetry group*** *if for all* $\sigma \in \mathcal{O}$ *there exists* $U \in \mathrm{U}(H)$ *such that*

$$U E_x U^* = E_{\sigma(x)} \quad \text{for all} \quad x \in M \qquad \text{and} \qquad UPU^{-1} = P.$$

The parameters $m$ and $f$ determine whether a fermion system in discrete space-time can have outer symmetry group $S_m$. In [11, Section 9] it is shown:

**Theorem 2.13.** *If the number of particles and the number of space-time points satisfy the relation*

$$1 < f < m - 1,$$

*there cannot exist a fermion system in discrete space-time with outer symmetry group* $S_m$*.*

Thus the original permutation symmetry of the system is spontaneously broken by the fermionic projector. This effect has been illustrated in [5].

Having discussed the appearing symmetries, we now regard the variational principle (2.1.8) on different operators. We first restrict the fermionic projectors to a special class:

**Definition 2.14.** *A fermionic projector* $P$ *is called* ***homogeneous****, if for all points* $x_0, x_1 \in M$ *there exists* $\sigma \in S_m$ *with* $\sigma(x_0) = x_1$ *and* $U \in \mathcal{G}$ *such that*

$$P(\sigma(x), \sigma(y)) = U P(x,y) U^* \quad \text{for all} \quad x, y \;\in M. \tag{2.1.15}$$

This class of fermionic projectors is of special physical interest as the vacuum should be described by a homogeneous fermionic projector. In particular, the discrete kernels $P(x,x)$ coincide in its eigenvalues and satisfy $\mathrm{Tr}(P(x,x)) = \frac{f}{m}$ for all $x \in M$. Thus an application of Theorem 2.6 yields that in this class the variational principle is well-defined, see [12, Theorem 2.5]:

**Theorem 2.15.** *Minimizing the action* (2.1.7) *by varying $P$ in the class of homogeneous fermionic projectors, the minimum is attained.*

The variational principle can further be considered on a more general class of operators: If $A$ is a self-adjoint operator on the inner product space $H$, we call $A$ **positive** if

$$\langle \xi \,|\, A\xi \rangle \geq 0 \quad \text{for all} \quad \xi \in H.$$

**Definition 2.16.** *A self-adjoint operator $P$ is called* ***of class*** $\mathcal{P}^f$ *if $-P$ is positive and $P$ satisfies the relations*

$$\mathrm{Tr}(P) = f \quad \textit{and} \quad \mathrm{rk}(P) \leq f.$$

**Theorem 2.17.** *The variational principle* (2.1.8) *considered for $P \in \mathcal{P}^f$ attains its minimum in $\mathcal{P}^f$.*

We refer to [12, Theorem 2.9] for the proof.

## 2.2 The Variational Principle in Matrix Formulation - the Particle Representation

The variational principle in discrete space-time can be reformulated as a matrix problem, which will be shown in Section 2.3, and which is denoted as the particle representation. The corresponding action principle on matrices can be introduced independent of the space-time setting as follows: Let $f, m \in \mathbb{N}$ be parameters with $m \geq f$ and $M = \{1, \ldots, m\}$. Let $(F_x)_{x \in M}$ be a family in $\mathrm{Mat}(f \times f, \mathbb{C})$ satisfying the properties

**(E)** for each $x \in M$ the matrix $F_x$ is hermitian with at most one positive and at most one negative eigenvalue, counted with algebraic multiplicities,

**(F1)** the family $(F_x)_{x \in M}$ is complete, i.e.

$$\sum_{x \in M} F_x \;=\; \mathbb{1}_f. \tag{2.2.16}$$

The matrix product $F_x F_y$ of matrices $F_x, F_y$ satisfying property (E) has rank at most two. This allows to adapt formula (2.1.9):

**Definition 2.18.** *Let $\lambda_\pm$ denote the non-trivial eigenvalues of $F_x F_y$, counted with algebraic multiplicities. Then the Lagrangian of $F_x, F_y$ is defined as*

$$\mathcal{L}[F_x, F_y] = \frac{1}{2}\Big(|\lambda_+| - |\lambda_+|\Big)^2. \tag{2.2.17}$$

The variational principle is stated as

$$\boxed{\textbf{minimize } \mathcal{S}[(F_x)_{x\in M}] = \sum_{x,y\in M} \mathcal{L}[F_x, F_y]} \tag{2.2.18}$$

varying $(F_x)_{x\in M}$ in the family of $f \times f$-matrices satisfying the properties (E) and (F1), keeping the parameters $f, m$ fixed.

We discuss the new setting: Introducing $A_{xy} := F_x F_y$ for $x, y \in M$, the Lagrangian can be rewritten using the spectral weight as $\mathcal{L}[F_x, F_y] = |A_{xy}^2| - \frac{1}{2}|A_{xy}|^2$. The product $F_x F_y$ of two hermitian matrices $F_x, F_y$ is in general not hermitian, but Proposition 2.8 yields that the eigenvalues of $F_x F_y$ lie symmetric relative to the real axis. This allows to adapt the notion of causality introduced in Definition 2.10.

The Lagrangian is in each argument homogeneous of degree two: if the matrices $F_1, F_2 \in \mathrm{Mat}(f \times f, \mathbb{C})$ satisfy property (E), it is

$$\mathcal{L}[\lambda F_1, F_2] = \mathcal{L}[F_1, \lambda F_2] = \lambda^2 \mathcal{L}[F_1, F_2] \quad \text{for all} \quad \lambda > 0. \tag{2.2.19}$$

Furthermore, the variational principle is $\mathrm{U}(f)$-invariant: if $V \in \mathrm{U}(f)$, a unitary transformation of the family $(F_x)_{x\in M}$

$$F_x \to V F_x V^\dagger \quad \text{for all} \quad x \in M, \tag{2.2.20}$$

yields a family of matrices satisfying the constraints (E) and (F1), and of the same action.

The properties (E) and (F1) are used in the next section to reconstruct a fermionic projector in discrete space-time. But it is also required to consider the variational principle (2.2.18) on a family $(F_x)_{x\in M}$ of hermitian matrices satisfying different properties. Keeping property (E), a supplementary property is needed to rule out trivial solutions. The property (F1) can be replaced be prescribing the non-trivial eigenvalues: For $\alpha, \beta \geq 0$, an alternate condition is:

**(F2)** For each $x \in M$ the non-trivial eigenvalues of $F_x$ are prescribed as $\alpha$ and $-\beta$.

**Definition 2.19.** *The family of matrices satisfying (E) and (F2) is denoted as* $\mathcal{F}$.

Property (F1) can be stated weaker:

**(F3)** The family $(F_x)_{x\in M}$ satisfies the trace constraint

$$\sum_{x\in M} \mathrm{Tr}(F_x) \;=\; f. \tag{2.2.21}$$

In the following section, we will show that the discrete space-time representation and the particle representation are equivalent, thus the existence of a minimizer of the variational principle (2.2.18) on matrices is equivalent to the already treated existence of a minimizer of the variational principle (2.1.8) in discrete space-time.

## 2.3 The Transition between the two Formulations

### 2.3.1 From the Space-Time to the Particle Representation

The variational principle in discrete space-time can be presented as a matrix problem via the following considerations: Let $(H, \langle .|. \rangle, (E_x)_{x \in M})$ be a discrete space-time with $m$ space-time points and let $f \leq m$.

**Definition 2.20.** *Let $\psi_1, \ldots, \psi_f \in H$ be an orthogonal system of $f$ negative vectors. Then the linear mapping*

$$\Psi \;:\; \mathbb{C}^f \to H, \quad u \mapsto \sum_{\alpha=1}^{f} \psi_\alpha u^\alpha \tag{2.3.22}$$

*is called **fermion matrix**. The **local fermion matrix** $\Psi_x$ is the restriction of $\Psi$ on the space-time point $x \in M$,*

$$\Psi_x = E_x \Psi : \mathbb{C}^f \to E_x(H), \quad u \mapsto \sum_{\alpha=1}^{f} (E_x \psi_\alpha)\, u^\alpha \;\;. \tag{2.3.23}$$

The adjoint $\Psi^*$ of a fermion matrix $\Psi$ is the unique mapping which satisfies

$$\langle\, \Psi\, u \,|\, \xi \,\rangle \;=\; (\, u \,|\, \Psi^* \, \xi \,)_{\mathbb{C}^f} \quad \text{for all} \quad u \in \mathbb{C}^f,\; \xi \in H$$

and is given by

$$\Psi^* : H \to \mathbb{C}^f, \quad u \mapsto \Big( \langle \psi_\alpha | u \rangle \Big)_{\alpha=1 \ldots f}. \tag{2.3.24}$$

Choosing the basis of $H$, where the inner product and the space-time projectors are represented as in (2.1.11) and (2.1.12), the adjoint is represented as $\Psi^* = \Psi^\dagger S$. The pseudo-orthonormality of the vectors $\psi_\alpha$ immediately yields the following Lemma.

**Lemma 2.21.** *i) Let $\Psi$ be a fermion matrix corresponding to the orthogonal negative vectors $\psi_1, \ldots, \psi_f$ in $H$.*

*a) The fermion matrix and its adjoint satisfy $\Psi^* \Psi = -\mathbb{1}_f$.*

*b) The linear operator $P$ defined by the composition*

$$P := -\Psi \Psi^* = -\sum_{\alpha=1}^{f} |\psi_\alpha\rangle \langle \psi_\alpha| \tag{2.3.25}$$

*is a fermionic projector of $f$ particles.*

*ii) Let $P$ be a fermionic projector of $f$ particles. Then each pseudo-orthonormal basis $\psi_1, \ldots, \psi_f$ of $P(H)$ defines a fermion matrix. A change of basis corresponds to a multiplication of $\Psi$ by a unitary matrix $V \in U(f)$, $\Psi \to \Psi V$.*

Here we used the Bra-ket notation to state the operator: For $\psi \in H$, the operator $Q := |\psi\rangle\langle\psi|$ is the linear operator on $H$ given by

$$Q(\xi) = \psi\langle\psi|\xi\rangle \quad \text{for all} \quad \xi \in H.$$

The discrete kernel and the closed chain of the fermionic projector $P$ can be rewritten using the local fermion matrices and its adjoint as

$$P(x,y) = -\Psi_x \, \Psi_y^*, \quad A_{xy} = \Psi_x \, \Psi_y^* \, \Psi_y \, \Psi_x^*. \tag{2.3.26}$$

The composition of the local fermion matrix with its adjoint yields the so-called correlation matrices:

**Definition 2.22.** *Let $P$ be a fermionic projector with fermion matrix $\Psi$. The* ***local correlation matrix*** *$F_x : \mathbb{C}^f \to \mathbb{C}^f$ at the space-time point $x \in M$ is defined by*

$$F_x = -\Psi^* \, E_x \, \Psi = -\Psi_x^* \, \Psi_x = \Big( - \langle \psi_\alpha | E_x \, \psi_\beta \rangle \Big)_{\alpha,\beta=1}^{f}. \tag{2.3.27}$$

These matrices are used to make the transition to particle representation, as the following two Lemmas show:

**Lemma 2.23.** *The family of local correlation matrices $(F_x)_{x \in M}$ corresponding to a fermionic projector $P$ satisfies the properties (E) and (F1).*

*Proof.* Lemma 2.21 and the completeness of the space-time projectors (2.1.1) yields the completeness of the family $(F_x)$. Let $x \in M$ be fixed. The matrix $F_x$ is hermitian since the operator $E_x$ is self-adjoint. Let $(u_i)_{i=1,\ldots,f}$ be an orthonormal basis in $\mathbb{C}^f$ of eigenvectors of $F_x$ with corresponding eigenvalues $\lambda_i \in \mathbb{R}$. Then the family $\{E_x \Psi u_i \,:\, u_i \notin \ker(F_x)\}$ is a linearly independent set of vectors in the vector space $E_x(H)$. Using the definition of $F_x$ and that the $E_x$ are projectors, one calculates

$$\lambda_i (u_i|u_i) = (u_i|F_x u_i) = (u_i|\Psi^* E_x \Psi u_i) = \langle E_x \Psi u_i | E_x \Psi u_i \rangle.$$

Since the inner product space $E_x(H)$ has signature $(1,1)$, we conclude that $F_x$ can have at most one positive and at most one negative eigenvalue. □

We remark that if the fermionic projector is also homogeneous, the family $(F_x)$ of local correlation matrices satisfies additionally the eigenvalue constraint $(F2)$.

**Lemma 2.24.** *Let $P$ be a fermionic projector with corresponding closed chains $A_{xy}$ and local correlation matrices $(F_x)_{x \in M}$. Then the Lagrangians coincide,*

$$\mathcal{L}[A_{xy}] = \mathcal{L}[F_x, F_y] \quad \textit{for all} \quad x, y \in M.$$

*Proof.* Expressing the closed chain via (2.3.26) with the local fermion matrices and using the commutation law (2.1.14) for the characteristic polynomial, one obtains

$$\det(F_x F_y - \lambda \mathbb{1}_f) = \lambda^{f-2} \det(\Psi_x \Psi_y^* \Psi_y \Psi_x^* - \lambda \mathbb{1}_2) = \lambda^{f-2} \det(A_{xy} - \lambda \mathbb{1}_2).$$

We conclude that the non-trivial eigenvalues of $F_x F_y$ and $A_{xy}$ and thus the Lagrangians coincide. □

In particular, the local correlation matrices yield the same action as the underlying fermionic projector.

The fermion matrix can be transformed without changing the action and the space-time structure via

$$\Psi \to U\, \Psi\, V^{-1} \quad \text{with} \quad U \in \mathcal{G},\ V \in \mathrm{U}(f). \tag{2.3.28}$$

The multiplication from the right by an element in $\mathrm{U}(f)$ corresponds to a change of the basis of $P(H)$ and does not change the fermionic projector $P$, whereas it unitary transforms the local correlation matrices via (2.2.20). The multiplication from the left by an element in $\mathcal{G}$ is just the gauge transformation of the corresponding fermionic projector $P$, which does not effect the local correlation matrices $(F_x)_{x \in M}$.

### 2.3.2 From the Particle to the Space-Time Representation

Having transferred the variational principle on fermionic projectors into a matrix problem, we now attend to the reverse task. In the proof, we adapt ideas from [2, Section 3].

**Proposition 2.25.** *Let $(H, \langle .|. \rangle, (E_x)_{x \in M})$ be a discrete space-time of $m$ space-time points and for $f \leq m$ let $(F_x)_{x \in M}$ be a family of matrices in $\mathrm{Mat}(f \times f, \mathbb{C})$ that satisfies (E) and (F1). Then there exists a fermionic projector $P$, whose local correlation matrices coincide with $(F_x)_{x \in M}$.*

*Proof.* Let $x \in M$ be fixed. According to property (E), there exist $\alpha_x, \beta_x \geq 0$ and $V_x \in \mathrm{U}(f)$ such that

$$V_x^\dagger F_x V_x = \mathrm{diag}(\alpha_x, -\beta_x, 0, \ldots, 0) =: D_x.$$

The signature matrix

$$\Sigma_x = \mathrm{diag}(1, -1, 0, \ldots, 0) \in \mathrm{Mat}(f \times f, \mathbb{C})$$

defines on $\mathbb{C}^f$ a possibly degenerate inner product $(.|\Sigma_x .)$ of signature $(1,1)$, where $(.|.)$ denotes the standard inner product on $\mathbb{C}^f$. Let $T_x : \mathbb{C}^f \to (E_x(H), \langle .|. \rangle)$ be a linear mapping which satisfies

$$\langle T_x u | T_x v \rangle = -(u | \Sigma_x v) \quad \text{for all} \quad u, v \in \mathbb{C}^f. \tag{2.3.29}$$

If $\xi_1, \xi_2 \in E_x(H) \subset H$ denotes a basis of $E_x(H)$ with $\langle \xi_1 | \xi_1 \rangle = 1$, $\langle \xi_2 | \xi_2 \rangle = -1$ and $\langle \xi_1 | \xi_2 \rangle = 0$, the operator $T$ may be defined as $T(e_1) = \xi_2$, $T(e_2) = \xi_1$ and $T(e_i) = 0$ for $i = 3, \ldots, f$ (where $e_i$ denotes the $i$-th unit vector in $\mathbb{C}^f$). Defining $\Psi_x$ as

$$\Psi_x := T_x \sqrt{|D_x|} V_x^\dagger : \mathbb{C}^f \longrightarrow E_x(H),$$

it is using (2.3.29) for $u, v \in \mathbb{C}^f$

$$(\, \Psi_x^* \, \Psi_x \, u \,|\, v) = \langle\, \Psi_x \, u \,|\, \Psi_x \, v \,\rangle = -\Big(\, \sqrt{|D_x|}\ V_x^\dagger\ u \;\Big|\; \Sigma_x\ \sqrt{|D_x|}\ V_x^\dagger\ v \Big) = -(\, F_x \, u \,|\, v).$$

We conclude that for each $x \in M$ there exists $\Psi_x : \mathbb{C}^f \to E_x(H)$ with $-\Psi_x^* \Psi_x = F_x$. We define the operator $\Psi$ by

$$\Psi = \bigoplus_{x \in M} \Psi_x : \mathbb{C}^f \to H, \quad u \mapsto \sum_{x \in M} \Psi_x u.$$

According to the identity constraint (F1), we obtain for $u, v \in \mathbb{C}^f$

$$\langle \Psi u \,|\, \Psi\, v \rangle = \Big\langle \sum_{x=1}^m \Psi_x\, u \,\Big|\, \sum_{y=1}^m \Psi_y\, v \Big\rangle = \sum_{x=1}^m \langle \Psi_x u \,|\, \Psi_x v \rangle = -\sum_{x=1}^m (u \,|\, F_x\, v) = -(u|v).$$

Consequently, $\Psi$ is a fermion matrix. By construction, the local correlation matrices of the corresponding fermionic projector $P = -\Psi\Psi^*$ coincide with the given family of matrices $(F_x)$. □

The question of uniqueness is treated in [33]. If the hermitian matrices $F_x$ are all non-zero, the local fermion matrix $\Psi_x$ which satisfies $-\Psi_x^* \Psi_x = F_x$ is unique up to gauge transformation $\Psi_x \to U_x \Psi_x$ with $U_x \in \mathrm{U}(E_x(H))$. But a zero local correlation matrix yields local fermion matrices and thus fermionic projectors which are not gauge equivalent.

If the family of matrices $(F_x)_{x \in M}$ satisfy (E) and the trace constraint (F3), a similar construction as in the above proof yields an operator of class $\mathcal{P}^f$.

## 2.4 General Remarks

We finally compare the two approaches. The approach in the particle representation is easier accessible. The invariance under the non-compact gauge group $\mathcal{G}$ is replaced by a compact $\mathrm{U}(f)$-invariance. But since there are fermionic projectors belonging to the same local correlation matrices which are not gauge equivalent, there occurs a loss of information.

The fermion matrix and thus the space-time representation is more appropriate for solving the variational principle numerically because the constraints can be implemented more conveniently. For a comparison of the different solutions and in order to decide whether the minimizers are gauge equivalent, it is reasonable to analyze the local correlation matrices corresponding to the minimizing fermionic projector.

We finally state properties which are valid for both settings, and start with a remark on the notion of causality:

**Lemma 2.26.** *If the fermionic projector $P$ solves the variational principle* (2.1.8)*, each space-time point is timelike separated from itself.*

*Proof.* Let $(F_x)_{x \in M}$ be the corresponding family of local correlation matrices. Since the eigenvalues of the hermitian matrix $F_x^2$ are real, the space-time point $x$ is either lightlike or timelike separated from itself. Assume there exists $y \in M$ which is lightlike separated from itself. Then the discrete kernel $P(y, y)$ is nilpotent, implying

that the corresponding local correlation matrix $F_y$ vanishes. The family $(F_x)_{x \in M}$ of local correlation matrices thus reduces to a set of only $m-1$ matrices and consequently corresponds to a fermionic projector in a space-time of $m-1$ space-time points, in contradiction to (2.1.10). □

We now state an important transformation of the Lagrangian. Since the Lagrangian of the closed chain $A_{xy}$ and of $F_x, F_y$ coincide, the lemma similarly applies in both settings.

**Lemma 2.27.** *Let $\mathcal{L}$ be the Lagrangian defined in* (2.2.17). *Then $\mathcal{L}$ is given as the positive part of a smooth function,*

$$\mathcal{L}[F_x, F_y] = \max\Big(0, \mathcal{D}[F_x F_y]\Big) \quad \text{where} \quad \mathcal{D}[F_x, F_y] = \mathrm{Tr}\Big((F_x F_y)^2\Big) - \frac{1}{2}\,\mathrm{Tr}\,(F_x F_y)^2\,. \tag{2.4.30}$$

*In the case $f = 2$, the function $\mathcal{D}$ can be expressed as*

$$\mathcal{D}[F_x, F_y] = \frac{1}{2}\mathrm{Tr}(F_x F_y)^2 - 2\det(F_x F_y). \tag{2.4.31}$$

*Proof.* Let $x, y \in M$ be fixed. After a unitary transformation (2.2.20), we can assume that $F_x = \mathrm{diag}(\alpha_x, -\beta_x, 0 \ldots, 0)$ with $\alpha_x, \beta_x \geq 0$. Let $\lambda_\pm$ denote the non-trivial eigenvalues of $F_x F_y$. Let $\tilde{F}_y$ denote the $2 \times 2$ leading principal submatrix, thus $\tilde{F}_y = (g_{ij})_{i,j=1,2}$ for $F_y = (g_{ij})_{i,j=1,\ldots,f}$. Then the eigenvalues of $\tilde{F}_x \tilde{F}_y$ coincide with the non-trivial eigenvalues of $F_x F_y$. Since the matrix $\tilde{F}_y$ is indefinite, it is $\det(\tilde{F}_y) \leq 0$. We obtain

$$\mathrm{Tr}(F_x F_y) \in \mathbb{R} \quad \text{and} \quad \det(\tilde{F}_x \tilde{F}_y) = -\alpha_x \beta_x \det(\tilde{F}_y) \geq 0$$

and conclude that either $\lambda_+$ and $\lambda_-$ are real and have the same sign or else build a complex conjugate pair. For the Lagrangian given by (2.2.17), this yields to the form

$$\mathcal{L}[F_x, F_y] = \max\left(0, \frac{1}{2}\,(\lambda_+ - \lambda_-)^2\right),$$

where the non-trivial argument can be expressed as

$$\frac{1}{2}\,(\lambda_+ - \lambda_-)^2 = \mathrm{Tr}\Big((F_x F_y)^2\Big) - \frac{1}{2}\,\mathrm{Tr}\,(F_x F_y)^2\,.$$

Finally one verifies the basic identity

$$\mathrm{Tr}(A^2) = \mathrm{Tr}(A)^2 - 2\det(A) \quad \text{for} \quad A \in \mathrm{Mat}(2 \times 2, \mathbb{C}). \qquad \square$$

In the case $y = x$, the function $\mathcal{L}$ and $\mathcal{D}$ coincide since

$$\mathcal{L}[F_x, F_x] = \mathcal{D}[F_x, F_x] = \frac{1}{2}\left(\alpha_x^2 - \beta_x^2\right)^2 \geq 0. \tag{2.4.32}$$

With regard to Definition 2.10, the space-time points $x, y \in M$ are spacelike separated if and only if $\mathcal{D}[F_x, F_y] < 0$, lightlike separated if and only if $\mathcal{D}[F_x, F_y] = 0$, and timelike separated if and only if $\mathcal{D}[F_x, F_y] > 0$. Thus the sign of the smooth function $\mathcal{D}$ determines the causal structure. The fact that $\mathcal{L}$ is the positive part of a smooth function causes interesting effects, and will be treated in a more general context in Chapter 6.

# 3 Geometry of Causal Fermion Systems

## 3.1 Identification with Vectors on the Sphere in the Case of two Particles

In order to analyze the structure of a fermion system in discrete space-time, it is helpful to visualize the fermionic projector. For this purpose, it is most convenient to work in the particle representation and regard the corresponding local correlation matrices.

In a system with only two particles, each local correlation matrix can be visualized as a vector in $\mathbb{R}^3$, as we now describe. We start with introducing the *Pauli-matrices*

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

and refer to [26, Chapter 9] for their properties. As the matrices $\mathbb{1}_2, \sigma^1, \sigma^2, \sigma^3$ are linearly independent, any $F \in \mathrm{Mat}(2 \times 2, \mathbb{C})$ can be written as

$$F \;=\; \rho\, \mathbb{1} + \vec{c} \cdot \vec{\sigma} = \rho\, \mathbb{1}_2 + c_1\, \sigma^1 + c_2\, \sigma^2 + c_3\, \sigma^3 \quad \text{with} \quad \rho \in \mathbb{C},\ \vec{c} \in \mathbb{C}^3. \tag{3.1.1}$$

Using the product identity for the Pauli matrices

$$\sigma^k \sigma^l = \delta_{kl} \mathbb{1} + i \sum_{m=1}^{3} \varepsilon_{klm} \sigma_m \quad \text{for} \quad k, l = 1, 2, 3 \tag{3.1.2}$$

(where $\varepsilon_{klm}$ denotes the antisymmetric symbol) and that the Pauli matrices are traceless, the coefficients are given by

$$\rho = \frac{1}{2} \mathrm{Tr}(F) \quad \text{and} \quad c_k = \frac{1}{2} \mathrm{Tr}(F \sigma^k) \quad \text{for} \quad k = 1, 2, 3.$$

The determinant and the eigenvalues $\lambda_\pm$ of $F$ are then calculated as

$$\det(F) = \rho^2 - \sum_{i=1}^{3} c_i^2 \quad \text{and} \quad \lambda_\pm = \rho \pm \sqrt{\sum_{i=1}^{3} c_i^2}. \tag{3.1.3}$$

We apply these considerations to hermitian matrices and obtain:

**Lemma 3.1.** *If $F \in \mathrm{Mat}(2 \times 2, \mathbb{C})$ is hermitian, $F$ can be expanded as*

$$F \;=\; \rho\, \mathbb{1}_2 + \vec{c} \cdot \vec{\sigma} \quad \text{with} \quad \rho \in \mathbb{R},\; \vec{c} \in \mathbb{R}^3, \tag{3.1.4}$$

*where the vector $\vec{c}$ is called* ***Bloch vector****. The eigenvalues $\lambda_\pm$ of $F$ are given by*

$$\lambda_\pm = \rho \pm \|\vec{c}\|. \tag{3.1.5}$$

Finally we examine transformations of the objects in (3.1.4): The group $\mathrm{SU}(2)$ is the universal covering group of $\mathrm{SO}(3)$, $\mathrm{SO}(3) \simeq \mathrm{SU}(2)/\{\pm \mathbb{1}_2\}$, where the Pauli matrices can be used to construct the twofold covering map, (see [24, Chapter 1]). Thus for each $V \in \mathrm{SU}(2)$ there exists a unique $R \in \mathrm{SO}(3)$ such that

$$V(\rho \mathbb{1}_2 + \vec{c} \cdot \vec{\sigma}) V^{-1} = \rho \mathbb{1}_2 + (R\vec{c}) \cdot \vec{\sigma} \quad \text{for all} \quad \rho \in \mathbb{R},\; \vec{c} \in \mathbb{R}^3, \tag{3.1.6}$$

concluding that a unitary transformation of a hermitian matrix $F$ causes a rotation of the corresponding Bloch vector. Conversely, a rotation of the Bloch vector causes a unitary transformation of the matrix.

Now let $(H, \langle .|. \rangle, (E_x)_{x \in M}, P)$ be a fermion system in discrete space-time with two particles. According to Lemma 3.1, each local correlation matrix $F_x \in \mathrm{Mat}(2 \times 2, \mathbb{C})$ can be assigned the parameter $\rho_x$ and the Bloch vector $\vec{c}_x$. Since each $F_x$ has non-positive determinant we get the relation

$$\|\vec{c}_x\| \;\geq\; |\rho_x| \quad \text{for all} \quad x \in M. \tag{3.1.7}$$

The completeness of the family $(F_x)$ yields

$$\sum_{x \in M} \rho_x = 1 \quad \text{and} \quad \sum_{x \in M} \vec{c}_x = 0. \tag{3.1.8}$$

According to formula (3.1.6), a unitary transformation (2.2.20) of the family of correlation matrices corresponds to a rotation of all Bloch vectors. If there is a system of parameters $\rho_x \in \mathbb{R}$ and vectors $\vec{c}_x \in \mathbb{R}^3$ which satisfy (3.1.8) and (3.1.7), then using Proposition 2.25 there exists a fermionic projector such that the corresponding local fermion matrices $F_x$ realize $\rho_x$ and $\vec{c}_x$. This fermionic projector, however, may not be unique, see [5, Example 4.3].

We now express the function $\mathcal{D}$ defined by (2.4.31) and thus the Lagrangian using the local traces and Bloch vectors of the local correlation matrices $F_x$:

**Lemma 3.2.** *For $x, y \in M$ let $F_x, F_y$ be decomposed as in* (3.1.4)*,*

$$F_x \;=\; \rho_x\, \mathbb{1}_2 + \vec{c}_x \cdot \vec{\sigma} \quad \text{and} \quad F_y \;=\; \rho_y\, \mathbb{1}_2 + \vec{c}_y \cdot \vec{\sigma}\,.$$

*Then the function $\mathcal{D}[F_x, F_y]$ defined in* (2.4.30) *is calculated as*

$$\mathcal{D}[F_x, F_y] = 2 \left[ \Big( \rho_x \rho_y + \vec{c}_x \cdot \vec{c}_y \Big)^2 - \Big( \rho_x^2 - \|\vec{c}_x\|^2 \Big) \Big( \rho_y^2 - \|\vec{c}_y\|^2 \Big) \right]. \tag{3.1.9}$$

*Proof.* For vectors $\vec{u}, \vec{v} \in \mathbb{R}^3$ it is using (3.1.2)

$$(\vec{u} \cdot \vec{\sigma})\ (\vec{v} \cdot \vec{\sigma}) = \vec{u} \cdot \vec{v}\ \mathbb{1}_2 + i\ (\vec{u} \times \vec{v}) \cdot \vec{\sigma},$$

where $\vec{u} \cdot \vec{v} = \sum_i u_i v_i$ denotes the standard dot product and $\times$ the standard cross product in $\mathbb{R}^3$. We obtain for the product of two matrices in Bloch representation the formula

$$F_x F_y = (\rho_x \rho_y + \vec{c}_x \cdot \vec{c}_y) \mathbb{1}_2 + (\rho_x \vec{c}_y + \rho_y \vec{c}_x + i\ (\vec{c}_x \times \vec{c}_y)) \cdot \vec{\sigma} =: \kappa\, \mathbb{1} + \vec{d} \cdot \vec{\sigma} \quad (3.1.10)$$

with $\kappa \in \mathbb{R}$, $\vec{d} \in \mathbb{C}^3$. Formula (3.1.3) yields the relations $\mathrm{Tr}(F_x F_y) = 2\kappa$ and $\det(F_x F_y) = \kappa^2 - \sum_i d_i^2$. Hence the function $\mathcal{D}$ can be rewritten as

$$D[F_x, F_y] = 2 \sum_{i=1}^{3} d_i^2 = 2\ \left( \|\rho_x \vec{c}_y + \rho_y \vec{c}_x\|^2 - \|\vec{c}_x \times \vec{c}_y\|^2 \right).$$

Finally we use $\|\vec{c}_x \times \vec{c}_y\|^2 = \|\vec{c}_x\|^2 \|\vec{c}_y\|^2 - (\vec{c}_x \cdot \vec{c}_y)^2$. □

In particular, it is $\mathcal{D}[F_x, F_x] = 8 \rho_x^2 \|\vec{c}_x\|^2 \geq 0$.

Any fermionic projector is completely described by the set of local traces and the Bloch vectors of different lengths. The lengths and local traces simplify if the local correlation matrices all coincide in its eigenvalues:

**Corollary 3.3.** *If the local correlation matrices $(F_x)$ all have the same eigenvalues $\alpha$ and $-\beta$, the parameters $\rho_x$ and Bloch vectors $\vec{c}_x$ satisfy the relation*

$$\rho_x = \frac{1}{2}(\alpha - \beta), \quad \|\vec{c}_x\| = \frac{1}{2}(\alpha + \beta) \quad \textit{for all} \quad x \in M. \quad (3.1.11)$$

Accordingly, all Bloch vectors have the same length and can be normed to vectors of length one using the same normalization constant. A family $(F_x)$ of matrices in $\mathcal{F}$ with prescribed eigenvalues can therefore be identified with a family of $m$ vectors in the Euclidean two-sphere $S^2 \subset \mathbb{R}^3$.

## 3.2 The Geometry of Fermion Systems with Prescribed Eigenvalues

### 3.2.1 Identification with Flag Manifolds

In the case of a higher number of particles, it is no longer possible to illustrate a arbitrary fermionic projector like we have done in the case of two particles by assigning a family of Bloch vectors. A family of $f \times f$-matrices with prescribed eigenvalues, however, can be identified with elements in a homogeneous space, namely a certain flag manifold, see below. Additionally, we can illustrate the family of matrices by assigning a family of Lorentz vectors.

We begin with introducing homogeneous spaces, using definitions and theorems stated in [21, Chapter 9] and [31, Chapter 3].

**Definition 3.4.** *A **homogeneous space** is a smooth manifold $M$ on which a Lie group $G$ operates smoothly and transitively.*

A special class of homogeneous spaces are quotients of Lie groups by closed Lie subgroups. Moreover each homogeneous space is diffeomorphic to such a quotient space, as the following two Theorems show:

**Theorem 3.5.** *[Construction Theorem] Let $H$ be a closed submanifold of the Lie group $G$. Then there exists a manifold structure on the quotient space $G/H$ such that*

*i) the projection*

$$\pi : G \to G/H, \quad x \to xH$$

*is a smooth submersion,*

*ii) with the action*

$$G \times G/H \to G/H, \quad (x, yH) \to (xy)H$$

*the space $G/H$ gets a $G$-homogeneous space.*

**Theorem 3.6.** *[Characterization Theorem] Let $M$ be a $G$-homogeneous space and $p \in M$.*

*i) The stabilizer $G_p$ is a closed subset of $G$.*

*ii) The mapping*

$$F : G/G_p \to M, \;\; g\,G_p \mapsto g \cdot p$$

*is an equivariant diffeomorphism.*

Here, a mapping $F : M \to N$ between $G$-homogeneous spaces $M, N$ is called *equivariant*, if $F(g \cdot x) = g \cdot F(x)$ for all $g \in G$ and $x \in M$.

We apply the above Theorems to the following basic example:

*Example* 3.7. The $(n-1)-$sphere $S^{n-1} \subset \mathbb{R}^n$ is a homogeneous space since $\mathrm{O}(n)$ acts transitively on $S^{n-1}$. The stabilizer of the north pole is $\mathrm{O}(n-1) \subset \mathrm{O}(n)$ and thus

$$S^{n-1} \simeq \mathrm{O}(n)/\mathrm{O}(n-1).$$

We now introduce the homogeneous spaces which we need in the following:

**Proposition 3.8.** *The **Stiefel manifold** $V_k(\mathbb{C}^n)$, defined as*

$$V_k(\mathbb{C}^n) = \{X \in \mathrm{Mat}(n \times k, \mathbb{C}) \;:\; X^\dagger X = \mathbb{1}_k\},$$

*is a compact $\mathrm{U}(n)$-homogeneous manifold of real dimension $2nk - k^2$ with*

$$V_k(\mathbb{C}^n) \simeq \mathrm{U}(n)/\mathrm{U}(n-k). \tag{3.2.12}$$

*Proof.* The group $\mathrm{U}(n)$ acts smoothly and transitively on $V_k(\mathbb{C}^n)$ via matrix multiplication. The stabilizer of the point $X = \left(\begin{smallmatrix} \mathbb{1}_k \\ 0 \end{smallmatrix}\right) \in V_k(\mathbb{C}^n)$ is

$$H = \left\{ \begin{pmatrix} \mathbb{1}_k & 0 \\ 0 & C \end{pmatrix} \;:\; C \in \mathrm{U}(n-k) \right\} \simeq \mathrm{U}(n-k).$$

According to Theorem 3.6, the space $V_k(\mathbb{C}^n)$ is diffeomorphic to $\mathrm{U}(n)/H$ . Since $\mathrm{U}(n)$ is a Lie group of real dimension $\dim(\mathrm{U}(n)) = n^2$, we conclude

$$\dim(V_k(\mathbb{C}^n)) = \dim(\mathrm{U}(n)) - \dim(\mathrm{U}(n-k)) = n^2 - (n-k)^2 = 2nk - k^2.$$

Since the mappings noted in Theorem 3.6 and 3.5 are smooth, the compactness of $\mathrm{U}(n)$ yields the compactness of $V_k(\mathbb{C}^n)$. □

In a similar way we can proof:

**Proposition 3.9.** *The* ***flag manifold*** $\mathcal{F}_{1,2}(\mathbb{C}^n)$*, defined as*

$$\mathcal{F}_{1,2}(\mathbb{C}^n) = \big\{ (U,V) \,|\, U \subset V \subset \mathbb{C}^n \text{ is a flag with } \dim_{\mathbb{C}} U = 1,\, \dim_{\mathbb{C}} V = 2 \big\},$$

*is a compact* $\mathrm{U}(n)$*-homogeneous manifold of real dimension* $4n-6$ *with*

$$\mathcal{F}_{1,2}(\mathbb{C}^n) \simeq \mathrm{U}(n)/(\mathrm{U}(1) \times \mathrm{U}(1) \times \mathrm{U}(n-2)) \tag{3.2.13}$$

*Proof.* The group $\mathrm{U}(n)$ acts smoothly and transitively on the space $\mathcal{F}_{1,2}(\mathbb{C})$ via multiplication on the basis vectors of the flag. The stabilizer of the flag $X = (\mathrm{span}(e_1) \subset \mathrm{span}(e_1, e_2))$ is the closed subset

$$H = \left\{ \begin{pmatrix} A_1 & & \\ & A_2 & \\ & & C \end{pmatrix} \;:\; A_i \in \mathrm{U}(1),\; C \in \mathrm{U}(n-2) \right\}.$$

According to Theorem 3.6, $\mathrm{U}(n)/H$ is diffeomorphic to $\mathcal{F}_{1,2}(\mathbb{C}^n)$. □

We here restricted on flag manifolds of type $(1,2)$. The flag manifold can be defined in general type by considering flags of the prescribed dimensions.

We transmit these considerations as follows: If $\mathcal{F}$ denotes the family of hermitian $f \times f$-matrices with prescribed eigenvalues $\alpha$ and $-\beta$, every $x \in \mathcal{F}$ is uniquely described by the corresponding one-dimensional eigenspaces $U$ and $V$ of $\alpha$ and $-\beta$, and the chain $U \subset (U \cup V)$ is an element of $\mathcal{F}_{1,2}(\mathbb{C}^f)$. Thus the space $\mathcal{F}$ can be identified with the flag manifold $\mathcal{F}_{1,2}(\mathbb{C}^f)$. Additionally, the elements in $\mathcal{F}$ can be represented as

$$\alpha\, |u)(u| - \beta\, |v)(v| \quad \text{for} \quad u, v \in \mathbb{C}^f,\; \|u\| = 1 = \|v\|,\; u \perp v. \tag{3.2.14}$$

The vectors $u, v$ are unique up to a phase. Due to the orthonormality, the matrix $V = (u, v) \in \mathrm{Mat}(f \times 2, \mathbb{C})$ is an element in the Stiefel manifold $V_2(\mathbb{C}^f)$. As the flag manifold is compact and the action is continuous, we can conclude that the variational principle on matrix formulation (2.2.18) restricted on $\mathcal{F}$ attains its minimum.

### 3.2.2 The Gramian and the Relation to Minkowski Space-Time

Beneath the identification with elements of homogeneous spaces, we can describe a family of local correlation matrices which coincide in its eigenvalues with a Gramian and identify the causal structure with the causal structure of Minkowski space-time. We refer to [19, Chapter 7.2] for the next Definition and Proposition:

**Definition 3.10.** *Let $V$ be a $n$-dimensional complex vector space endowed with a positive definite inner product $\langle .|. \rangle$. The Gramian of the vectors $w_1, \ldots, w_k$ in $V$ with respect to $\langle .|. \rangle$ is the matrix $G = (g_{ij})_{i,j=1,\ldots,k} \in \mathrm{Mat}(k \times k, \mathbb{C})$ defined by*

$$g_{ij} = \langle w_i | w_j \rangle \quad \text{for} \quad i, j = 1, \ldots, k. \tag{3.2.15}$$

The Gramian matrix has the following fundamental property:

**Proposition 3.11.** *Let $G$ be the Gramian of the vectors $w_1, \ldots, w_k$ with respect to the positive inner product $\langle .|. \rangle$. Then $G$ is a hermitian, positive semi-definite matrix. The rank of $G$ coincides with the maximum number of linearly independent vectors in the set $\{w_1, \ldots, w_k\}$.*

On the other hand, each hermitian positive semi-definite matrix can be regarded as a Gramian:

**Proposition 3.12.** *Let $G \in \mathrm{Mat}(n \times n, \mathbb{C})$ be a hermitian, positive semi-definite matrix with $\mathrm{rk}\, G = k \leq n$. Then there exists a matrix $W \in \mathrm{Mat}(k \times n, \mathbb{C})$ of rank $k$ such that $G = W^\dagger W$.*

*Proof.* Since $G$ is hermitian, there exists $U \in \mathrm{U}(n)$ and a diagonal matrix $D \in \mathrm{Mat}(n \times n, \mathbb{C})$ such that $UDU^{-1} = G$, where the entries of $D$ are ordered as $d_{ii} > 0$ for $1 \leq i \leq k$, $d_{ii} = 0$ else. With the matrix $B = (b_{ij}) \in \mathrm{Mat}(k \times n, \mathbb{C})$ given as $b_{ij} = \sqrt{d_{ij}}$ for $i = 1, \ldots, k$, $j = 1, \ldots, n$, we define $W := BU^{-1}$. □

Defining $w_i := We_i \in \mathbb{C}^k$ for $i = 1, \ldots, n$, the matrix $G$ is the Gramian of the vectors $w_1, \ldots, w_n$ with respect to the standard Euclidean scalar product on $\mathbb{C}^k$. The vectors $w_1, \ldots, w_n$ span $\mathbb{C}^k$.

Now let $(F_x)_{x \in M}$ be a family in $\mathcal{F}$. According to (3.2.14), each element $F_x$ can be identified with two orthonormal vectors $u_x, v_x \in \mathbb{C}^f$. Ordering the $2m$ vectors as

$$(w_1, \ldots, w_{2m}) := (u_1, v_1, u_2, v_2, \ldots, u_m, v_m), \tag{3.2.16}$$

we define $G = (g_{ij}) \in \mathrm{Mat}(2m \times 2m, \mathbb{C})$ as the Gramian of the vectors $w_1, \ldots, w_{2m}$ with respect to the standard Euclidean scalar product $(.|.)$ in $\mathbb{C}^{2m}$. We partition the matrix $G$ into $2 \times 2$ matrices

$$G = \begin{pmatrix} G_{11} & \ldots & G_{1m} \\ \vdots & \ddots & \vdots \\ G_{m1} & \ldots & G_{mm} \end{pmatrix}, \tag{3.2.17}$$

where for $x, y \in M$ the matrix $G_{xy} \in \mathrm{Mat}(2 \times 2, \mathbb{C})$ is given by

$$G_{xy} = \begin{pmatrix} g_{2x-1,2y-1} & g_{2x-1,2y} \\ g_{2x,2y-1} & g_{2x,2y} \end{pmatrix}.$$

Due to the orthonormality of the vectors $u_x, v_x$, it is $G_{xx} = \mathbb{1}_2$ for all $x \in M$. The rank of the Gramian $G$ is determined by the number of linearly independent vectors in the set $\{w_1, \ldots, w_k\}$.

**Definition 3.13.** *Let $(F_x)_{x \in M}$ in $\mathrm{Mat}(f \times f, \mathbb{C})$ be a family of matrices. We call the family **regular**, if*

*i) for all $x \in M$ it is $F_x \in \mathcal{F}$,*

*ii) for $F_x$ represented as in (3.2.14), the vectors $u_1, v_1, \ldots, u_m, v_m$ span $\mathbb{C}^f$.*

*A discrete fermion system $(H, \langle .|. \rangle, (E_x)_{x \in M}, P)$ is called **regular**, if its local correlation matrices $(F_x)$ are regular.*

According to Proposition 3.11, the Gramian $G$ according to a regular family of matrices has rank $f$.

A regular family of matrices is completely described by the Gramian:

**Lemma 3.14.** *Let $G \in \mathrm{Mat}(2m \times 2m, \mathbb{C})$ be hermitian positive semi-definite with $\mathrm{rk}\, G = f$ be partitioned as in (3.2.17) with $G_{xx} = \mathbb{1}_2$ for all $x \in M$. Then there exists a regular family $(F_x)$ whose corresponding Gramian coincides with $G$.*

*Proof.* According to Proposition 3.12, there exists $W \in \mathrm{Mat}(f \times 2m, \mathbb{C})$ such that

$$W^\dagger W = G \tag{3.2.18}$$

Ordering the columns $w_i$ of $W$ as in (3.2.16), for each $x \in M$ we can define the matrix $F_x$ via (3.2.14). □

The family $(F_x)$ does not satisfy the identity constraint but choosing $\alpha = \frac{1}{m} + \beta$ it satisfies the trace constraint and thus can be used to reconstruct an operator of class $\mathcal{P}^f$.

For the construction of the Gramian of a regular fermion system, let the matrix $W \in \mathrm{Mat}(f \times 2m, \mathbb{C})$ be given in Block matrix notation as $W = (W_1 | \ldots | W_m)$ with $W_x \in V_2(\mathbb{C}^f)$. Then the Gramian $G$ given as

$$G_{xy} = W_x^\dagger W_y \quad \text{for all} \quad x, y \in M \tag{3.2.19}$$

satisfies the requirements of the Lemma above. Defining $R, s \in \mathrm{Mat}(2 \times 2, \mathbb{C})$ as

$$R = \begin{pmatrix} \sqrt{\alpha} & 0 \\ 0 & \sqrt{\beta} \end{pmatrix} \quad \text{and} \quad s = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma^3, \tag{3.2.20}$$

the local correlation matrices can be obtained via

$$F_x = W_x\, R\, s\, R\, W_x^\dagger \quad \text{for} \quad x \in M.$$

For the connection to Minkowski space-time, we note that the matrix $s$ is a signature matrix and thus defines an inner product of signature $(1,1)$ on $\mathbb{C}^2$. A matrix $A \in \mathrm{Mat}(2\times 2, \mathbb{C})$ is called *$s$-self-adjoint*, if it is self-adjoint with regard to the inner product $(.|s.)_{\mathbb{C}^2}$ or using (2.1.13) equivalently $sA^\dagger s = A$. A $s$-self-adjoint matrix can be represented in analogy to the Bloch representation (3.1.4) by a vector in $\mathbb{R}^{1,2}$, where $\mathbb{R}^{1,2}$ is the three-dimensional Minkowski space, i.e. $\mathbb{R}^3$ endowed with the inner product

$$\langle\langle \vec{v}, \vec{v} \rangle\rangle = v_0^2 - v_1^2 - v_2^2 \quad \text{for} \quad \vec{v} = \begin{pmatrix} v_0 \\ v_1 \\ v_2 \end{pmatrix} \in \mathbb{R}^3.$$

**Lemma 3.15.** *If $A \in \mathrm{Mat}(2\times 2, \mathbb{C})$ is $s$-self-adjoint, $A$ can be decomposed as*

$$A = \rho \mathbb{1}_2 + i v_1 \sigma^1 + i v_2 \sigma^2 + v_0 \sigma^3 \quad \textit{with} \quad \rho \in \mathbb{R},\ \vec{v} \in \mathbb{R}^{1,2}. \tag{3.2.21}$$

*The vector $\vec{v} \in \mathbb{R}^{1,2}$ given by (3.2.21) is called **Lorentz vector** of $A$. The eigenvalues $\lambda_\pm$ of $A$ are given by*

$$\lambda_\pm = \rho \pm \sqrt{\langle\langle \vec{v}, \vec{v} \rangle\rangle}, \tag{3.2.22}$$

*Proof.* Representing the matrix $A$ as in (3.1.1), it is $\rho, c_3 \in \mathbb{R}$. With regard to (3.1.2), for $k = 1, 2$ it is $s\sigma^k s = -\sigma^k$, concluding

$$\overline{\mathrm{Tr}(A\sigma^k)} = \mathrm{Tr}\left((A\sigma^k)^\dagger\right) = \mathrm{Tr}(sAs\sigma^k) = -\mathrm{Tr}(A\sigma^k),$$

which proves formula (3.2.21). Formula (3.1.3) completes the proof. □

With $A = (a_{ij})$ the coefficients are given by

$$\rho = \frac{1}{2}\left(a_{11} + a_{22}\right), \quad \vec{v} = \frac{1}{2}\begin{pmatrix} \mathrm{Tr}(A\sigma^3) \\ -i\,\mathrm{Tr}(A\sigma^1) \\ -i\,\mathrm{Tr}(A\sigma^2) \end{pmatrix} = \begin{pmatrix} \frac{1}{2}(a_{11} - a_{22}) \\ \mathrm{Im}(a_{12}) \\ \mathrm{Re}(a_{12}) \end{pmatrix} \in \mathbb{R}^{1,2}. \tag{3.2.23}$$

We apply the above Lemma on the Gramian as follows:

**Lemma 3.16.** *Let $G$ be a Gramian of a regular fermion system. For space-time points $x, y \in M$ let $L_{xy} \in \mathrm{Mat}(2\times 2, \mathbb{C})$ be defined as*

$$L_{xy} = R\, G_{xy}\, R\, s\, R\, G_{xy}^\dagger\, R\, s. \tag{3.2.24}$$

*Then $L_{xy}$ satisfies the following properties:*

*i) $L_{xy}$ is $s$-self-adjoint with $\det(L_{xy}) \geq 0$.*

*ii) The eigenvalues of $L_{xy}$ coincide with the non-trivial eigenvalues of $F_x F_y$.*

*Proof.* The second statement is again an application of Proposition 2.1.14. □

The $s$-self-adjoint matrix $L_{xy}$ can be assigned a scalar $\rho_{xy}$ and a Lorentz vector $\vec{v}_{xy} \in \mathbb{R}^{1,2}$ according to (3.2.21). In particular it is

$$L_{xx} = \begin{pmatrix} \alpha^2 & 0 \\ 0 & \beta^2 \end{pmatrix}, \quad \vec{v}_{xx} = \frac{1}{2}(\alpha^2 - \beta^2) \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \tag{3.2.25}$$

and the matrices satisfy $L_{xy} = sL_{yx}s$. Since $F_xF_y$ and $L_{xy}$ coincide in its non-trivial eigenvalues, the argument function $\mathcal{D}$ of the Lagrangian given by (2.4.30) can be rewritten as

$$\mathcal{D}[F_x, F_y] = 2\, \langle\langle \vec{v}_{xy}, \vec{v}_{xy} \rangle\rangle. \tag{3.2.26}$$

This implies that the notion of causality imposed in Definition 2.10 coincides with the usual notion of causality on the flat Minkowski space-time $\mathbb{R}^{1,2}$, as the Minkowski vector $\vec{v}_{xy} \in \mathbb{R}^{1,2}$ is timelike/lightlike/spacelike if and only if the space-time points $x, y$ are timelike/lightlike/spacelike separated.

In the special case that one of the prescribed eigenvalue vanishes, e.g. $\beta = 0$, each matrix $F_x \in \mathcal{F}$ can similar to (3.2.14) be described by a single vector $u_x \in \mathbb{C}^f$ with $\|u_x\| = 1$ via $F_x = \alpha\, |u_x)(u_x|$. This implies that the matrices $L_{xy}$ simplify to

$$L_{xy} = \alpha^2 |(u_x|u_y)|^2 \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},$$

which implies using formula (3.2.23) a trivial causal structure:

**Corollary 3.17.** *In the case $\beta = 0$, the Minkowski vectors $\vec{v}_{xy}$ for $x, y \in M$ lie on a line in one part of the light-cone, and are given by*

$$\vec{v}_{xy} = \frac{1}{2}\alpha^2 |(u_x|u_y)|^2 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}. \tag{3.2.27}$$

Thus in this special case, all Lorentz vectors thus lie on a line in one part of the open light-cone or else vanish.

To conclude, the Gramian yields a way to construct a regular family. The Lorentz vectors yield a geometric access to a homogeneous fermionic projector for an arbitrary number of particles and a tool to illustrate the causal relations. For each point $x \in M$, there is a set of Lorentz vectors $(\vec{v}_{xy})_{y \in M}$, which encodes the causal relations of the space-time. The family of Lorentz vectors for all base points $x \in M$ contains information about the symmetry of the system.

# 4 Numerical and Analytical Results for Minimizing Fermionic Projectors in Discrete Space-Time

## 4.1 Analytical Calculations for Special Cases

We now approach the task of solving the action principle on fermionic projectors in space-time representation (2.1.8). We begin by studying systems of only few space-time points and few particles in more detail and hence generalize the results of [5] and [25] to systems with more than two particles. In special cases, one can calculate analytically the minimal action of the variational principle (2.1.8). For the representation of the operators, we always use the basis such that the signature matrix and the space-time projectors are represented as in (2.1.11) and (2.1.12). We start with fermion systems in discrete space-time of only one particle:

**Proposition 4.1.** *The minimal action in a space-time consisting of $m$ space-time points and only one particle is given by*

$$\mathcal{S}_{\min} = \frac{1}{2m^2}. \tag{4.1.1}$$

*The minimizing fermionic projector is unique up to gauge transformation represented by*

$$P(x,y) = \frac{1}{m} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{for all} \quad x, y \in M. \tag{4.1.2}$$

*Proof.* According to Lemma 2.21, the fermionic projector according to the fermion matrix $\Psi = \psi_1$ for $\psi_1 \in H$ with $\langle \psi_1 | \psi_1 \rangle = -1$ is given by $P = -|\psi_1\rangle\langle\psi_1|$. The local traces of the fermionic projector simplify to

$$\rho_x = \mathrm{Tr}\big(P(x,x)\big) = -\langle E_x \psi_1 | E_x \psi_1 \rangle.$$

In view of Lemma 2.27, the Lagrangian $\mathcal{L}$ simplifies to

$$\mathcal{L}[A_{xy}] = \frac{1}{2}\mathrm{Tr}(A_{xy})^2 = \frac{1}{2}\mathrm{Tr}(E_x P E_y P E_x) = \frac{1}{2}\langle \psi_1 | E_x \psi_1 \rangle \langle \psi_1 | E_y \psi_1 \rangle = \frac{1}{2}\rho_x \rho_y,$$

where we used the invariance of the trace under cyclic permutations. Consequently, the action can be transformed to

$$\mathcal{S}[P] = \frac{1}{2} \sum_{x,y \in M} \rho_x^2 \rho_y^2 = \frac{1}{2} \left( \sum_{x \in M} \rho_x^2 \right)^2.$$

Applying the Cauchy-Schwarz inequality yields

$$1 = \left( \sum_{x \in M} \rho_x \right)^2 \leq \left( \sum_{x \in M} 1 \right) \left( \sum_{x \in M} \rho_x^2 \right),$$

where we used the relation (2.1.5) for the equation on the left. We conclude that

$$\frac{1}{2m^2} \leq \mathcal{S}[P].$$

Equality holds if and only if the two vectors $(\rho_x)_{x \in M}$ and $(1)_{x \in M}$ in $\mathbb{R}^m$ are linearly dependent, thus

$$\rho_x = \frac{1}{m} \quad \text{for all} \quad x \in M.$$

According to the operation properties of $\mathrm{U}(1,1)$ acting on $\mathbb{C}^2$, see [25, Chapter 3], for each $x \in M$ there exists $U \in \mathrm{U}(1,1)$ such that $U\Psi_x$ has the form $\frac{1}{\sqrt{m}} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$, concluding that the fermionic projector is represented as in (4.1.2). □

In the case of one particle, the minimizer is completely delocalized, since it has the same probability to be at any space-time point. Since the eigenvalues of $A_{xy}$ are $\frac{1}{m^2}$ and 0, all space-time points are timelike separated.

In a space-time with more than one particle, an explicit calculation of the action is hardly possible in general. As the Lagrangian is non-negative, the action (2.1.7) can be estimated by just summing over the diagonal entries,

$$\mathcal{S}[P] = \sum_{x,y \in M} \mathcal{L}[A_{xy}] \geq \sum_{x \in M} \mathcal{L}[A_{xx}], \tag{4.1.3}$$

where equality holds if and only if $\mathcal{L}[A_{xy}]$ vanishes for all $x \neq y$. We can estimate the diagonal entries as follows:

**Lemma 4.2.** *Let $(H, \langle .|. \rangle, (E_x), P)$ be a discrete fermion system of $m$ space-time points and $f$ particles. Then the diagonal entries of the action can be estimated by*

$$\sum_{x \in M} \mathcal{L}[A_{xx}] \geq \frac{f^4}{2m^3}, \tag{4.1.4}$$

*where equality holds if and only if the local correlation matrices are rank-one matrices with $\mathrm{Tr}(F_x) = \frac{f}{m}$ for all $x \in M$.*

*Proof.* Let $(F_x)_{x \in M}$ be the family of local correlation matrices of $P$ and $\alpha_x, -\beta_x$ denote the non-negative, non-positive eigenvalue of $F_x$. Using the identity constraint (2.2.16) and twice the Cauchy-Schwarz inequality, one obtains

$$f = \mathrm{Tr}(\sum_{x \in M} F_x) = \sum_{x \in M} (\alpha_x - \beta_x) \overset{(\times)}{\leq} \left( \sum_{x \in M} 1 \right)^{3/4} \left( \sum_{x \in M} (\alpha_x - \beta_x)^4 \right)^{1/4}.$$

By Definition, the Lagrangian on $x \in M$ is given by

$$\mathcal{L}[F_x, F_x] = \frac{1}{2} \left(\alpha_x^2 - \beta_x^2\right)^2$$

and can be estimated as

$$(\alpha_x - \beta_x)^4 \overset{(\star)}{\leq} (\alpha_x - \beta_x)^2 (\alpha_x + \beta_x)^2 = 2\mathcal{L}[F_x F_x].$$

Combining these two inequalities, one obtains the estimate

$$\frac{f^4}{2m^3} \leq \sum_{x \in M} \mathcal{L}[F_x, F_x].$$

Equality in $(\times)$ holds if and only the two vectors $(\alpha_x - \beta_x)_x$ and $(1)_x$ are linearly dependent, yielding $\alpha_x - \beta_x = \frac{f}{m}$ for all $x \in M$. Equality in $(\star)$ holds if and only if $\alpha_x \beta_x = 0$. Therefore the minimal contribution of the diagonal entries $\mathcal{L}[F_x, F_x]$ is attained in the case $\beta_x = 0 \quad \text{and} \quad \alpha_x = \frac{f}{m} \quad \text{for all} \quad x \in M.$ □

With regard to (4.1.3), we conclude that the minimal action can be estimated by

$$\mathcal{S}_{\min} \geq \frac{f^4}{2m^3}, \tag{4.1.5}$$

If there are exactly as many particles as space-time points, the lower bound of (4.1.5) is attained:

**Proposition 4.3.** *In the case $m = f$, the minimal action is given by*

$$\mathcal{S}_{\min} = \frac{f}{2}. \tag{4.1.6}$$

*The minimizing fermionic projector is unique up to gauge transformation represented as*

$$P(x,x) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \text{ for all } x \in M, \quad P(x,y) = 0 \text{ for all } x \neq y.$$

*Proof.* Let $(F_x)_{x \in M}$ be a family of rank-one matrices with $\mathrm{Tr}(F_x) = \frac{f}{m}$, given by

$$F_x = |u_x)(u_x| \quad \text{for} \quad u_x \in \mathbb{C}^f, \quad \|u_x\|^2 = \frac{f}{m}.$$

Since the product $F_x F_y = |u_x)(u_x|u_y)(u_y|$ is of rank at most one, the Lagrangian simplifies to

$$\mathcal{L}[F_x, F_y] = \frac{1}{2} |(u_x|u_y)|^4 \quad \text{for} \quad x, y \in M.$$

The Lagrangian vanishes for all distinct points if and only if the vectors $(u_x)_{x \in M}$ in $\mathbb{C}^f$ are mutually orthogonal. According to Lemma 4.2, the corresponding fermionic projector minimizes the action. The fermion matrix to the $m$ orthogonal negative vectors $\psi_x = e_x \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ (where $e_x$ denotes the $x$-th unit vector in $\mathbb{C}^m$) yields the up to gauge transformation unique fermionic projector $P$. □

The fermionic projector has maximal outer symmetry group $S_m$. All distinct points are lightlike separated. Each particle in the minimizing discrete fermion system is localized at one space-time point.

Considering the proof of Proposition 4.3, in the case $m > f$ there can not exist a fermionic projector such that all distinct points are lightlike or spacelike separated. Thus the action is always strictly larger than the sum of the diagonal entries,

$$\mathcal{S}_{\min} > \sum_{x \in M} \mathcal{L}[A_{xx}] \geq \frac{f^4}{2m^3} \quad \text{for} \quad m > f.$$

## 4.2 The Numerical Approach to Solve the Variational Principle in Discrete Space-time

### 4.2.1 The Augmented Lagrangian Method for Solving Nonlinear Constrained Optimization Problems

Since an analytic calculation may not be possible in general, we solve the variational principle (2.1.8) numerically. In the chosen basis, the action can be expressed as an optimization problem on the fermion matrix

$$\min_{\Psi \in \mathrm{Mat}(2m \times f, \mathbb{C})} \mathcal{S}[\Psi] \quad \text{subject to} \quad \Psi^\dagger S \Psi = -\mathbb{1}_f. \tag{4.2.7}$$

The minimization problem is a non-linear optimization problem with equality constraints, see [22, Chapter 15]. Such problems may in general be given as

$$\min_{x \in \mathbb{R}^n} \quad f(x) \quad \text{subject to} \quad r_i(x) = 0 \quad \text{for} \quad i \in \mathcal{E},$$

where $\mathcal{E} = \{1, \ldots, m\}$ is the set of equality restrictions and $f, r_i : \mathbb{R}^n \to \mathbb{R}$ are the objective and constraint functions.

Good results in our setting were attained by using the *method of augmented Lagrangian multipliers,* see [22, Chapter 17]. The basic idea is to solve instead of the original problem a series of unconstrained optimization problems, where the constraints appear as additional terms in the target function. In the quadratic penalty method, one minimizes in each step the penalty function

$$Q(x; \mu) = f(x) + \frac{\mu}{2} \sum_{i \in \mathcal{E}} r_i^2(x),$$

where the parameter $\mu > 0$ increases successively. This method was used and discussed in [25] to construct numerical solutions for small systems. Since the systems now under consideration get larger, the disadvantages of this method, like ill-conditioning and high run-time, appear badly and thus this method is no longer appropriate.

The augmented Lagrangian method combines the quadratic penalty method with the method of Lagrangian multipliers. Thus the augmented Lagrangian is defined as

$$\mathcal{L}_A(x, \lambda; \mu) = f(x) - \sum_{i \in \mathcal{E}} \lambda_i \, r_i(x) + \frac{\mu}{2} \sum_{i \in \mathcal{E}} r_i^2(x) \tag{4.2.8}$$

with the Lagrangian multiplier $\lambda \in \mathbb{R}^m$ and the penalty parameter $\mu > 0$. As the optimality condition is

$$0 \approx \nabla_x \mathcal{L}_A(x, \lambda; \mu) \;=\; \nabla f(x) - \sum_{i \in \mathcal{E}} [\lambda_i - \mu \, r_i(x)] \, \nabla r_i(x),$$

in each step the Lagrangian multiplier shall be replaced by $\lambda_i^{k+1} \;=\; \lambda_i^k - \mu_k \, r_i(x_k)$. This leads to the

**Algorithm 4.4.** *Augmented Lagrangian method*

***Start:*** $\mu_0 > 0$ , $\tau_0 > 0$ , $x_0^s \in \mathbb{R}^n$, $\lambda^0 \in \mathbb{R}^m$.

***for*** $k = 0, 1, 2, \ldots$

*i) Find local minimizer $x_k$ of $\mathcal{L}_A(., \lambda^k; \mu_k)$, starting at $x_k^s$.*
*STOP if $\|\nabla_x \mathcal{L}_A(x_k, \lambda^k; \mu_k)\| \leq \tau_k$*

*ii) If $x_k$ satisfies final convergence test STOP, end (if).*
*Set*

$$\lambda_i^{k+1} = \lambda_i^k - \mu_k r_i(x_k) \; , \quad x_{k+1}^s = x_k \; .$$

*Choose $\mu_{k+1} \geq \mu_k$, $\tau_{k+1} < \tau_k$, $k \leftarrow k + 1$.*

The tolerance $\tau_k$ determines the acceptance of a point as local minimum of the augmented Lagrangian function. The penalty parameter $\mu_k$ forces the iterated solutions into the feasible region. To ensure convergence, it is not required that $\mu_k \to \infty$, but the augmented Lagrangian method expires a local minimizer if $\mu_k$ is larger than a threshold value. The iterate $x_k$ will be accepted as final solution if the constraint functions at this point are satisfied in the accuracy of calculation.

It remains performing the local minimization in step i). Thus we now consider a nonlinear unconstrained minimization problem

$$\min_{x \in \mathbb{R}^n} \quad f(x),$$

where $f \in C^1(\mathbb{R}^n)$. We will use the *nonlinear conjugate gradient method*, which applies the conjugate gradient method to nonlinear optimization problems, see [22, Chapter 5] and [25]. This algorithm is implemented as follows, using the short notation $f_k = f(x_k)$ and $\nabla f_k = \nabla f(x_k)$.

**Algorithm 4.5.** *Fletcher-Reeves method*

***Start:*** $x_0 \in \mathbb{R}^n$, $p_0 = -\nabla f_0$, $\tau > 0$, $\hat{\alpha} > 0$, $\rho \in (0, 1)$, $c \in (0, 1)$, $\alpha \leftarrow \hat{\alpha}$.

**for** $k = 0, 1, 2, \ldots$

**if** $|\nabla f_k| < \tau$ *STOP, end (if)*

**while** $f(x_k + \alpha p_k) \leq f(x_k) + c\,\alpha\,(\nabla f_k)^t\, p_k$ *set* $\alpha \leftarrow \rho\,\alpha$

**set**

$$\begin{aligned} x_{k+1} &= x_k + \alpha p_k \\ \beta_{k+1} &= \frac{(\nabla f_{k+1})^t\, \nabla f_{k+1}}{(\nabla f_k)^t\, \nabla f_k} \\ p_{k+1} &= -\nabla f_{k+1} + \beta_{k+1} p_k \end{aligned}$$

$k \leftarrow k+1$, $\alpha \leftarrow \hat{\alpha}$ .

The choice of a suitable stepsize $\alpha$ is implemented in the while loop with the back tracking line search. This method realizes the Wolfe conditions the step size must satisfy and ends after a finite number of steps.

### 4.2.2 Application to Causal Variational Principles

We use the augmented Lagrangian method with the Fletcher-Reeves method to solve the variational principle in discrete space-time (4.2.7), see Appendix A, despite the fact that the function $\mathcal{L}$ and thus $\mathcal{S}$ is non-smooth, but since there is only one point where $\mathcal{L}$ is non-smooth, one might expect convergence. Indeed, the augmented Lagrangian method stops at a local minimum after a few steps of locally minimizing the unconstrained minimization and updating the values $\lambda_k, x_k$ in Algorithm 4.4. To explain the notation used in Appendix A, we write $\Psi \in \mathrm{Mat}(2m \times f, \mathbb{C})$ as

$$\Psi = \begin{pmatrix} t_{11} & \ldots & t_{1f} \\ u_{11} & \ldots & u_{1f} \\ \vdots & \ddots & \vdots \\ t_{m1} & \ldots & t_{mf} \\ u_{m1} & \ldots & u_{mf} \end{pmatrix} = T \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} + U \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{4.2.9}$$

where $T = V + iW$, $U = X + iY$. As $\Psi$ satisfies $\Psi^* \Psi = -\mathbb{1}_f$, due to the symmetry there are $\frac{f^2 - f}{2}$ constraint functions, namely

$$\begin{aligned} r_{ij}(V, W, X, Y) &= \sum_k -v_{ki} v_{kj} - w_{ki} w_{kj} + x_{ki} x_{kj} + y_{ki} y_{kj} \\ r_{ij}(V, W, X, Y) &= \sum_k -v_{ki} w_{kj} + w_{ki} v_{kj} + x_{ki} y_{kj} - y_{ki} x_{kj} \end{aligned}$$

for $i < j$ realizing the orthogonality of distinct columns, and

$$r_{ii}(V, W, X, Y) = \sum_k -v_{ki}^2 - w_{ki}^2 + x_{ki}^2 + y_{ki}^2 - 1$$

realizing the normalization. The increase of the tolerance and the penalty parameter in Alg. 4.4 is realized by multiplication with a positive scalar

$$\tau_k = \rho\,\tau_k \quad \text{and} \quad \mu_{k+1} = \gamma\,\mu_k \quad \text{where} \quad \rho > 1,\ \gamma \in (0, 1).$$

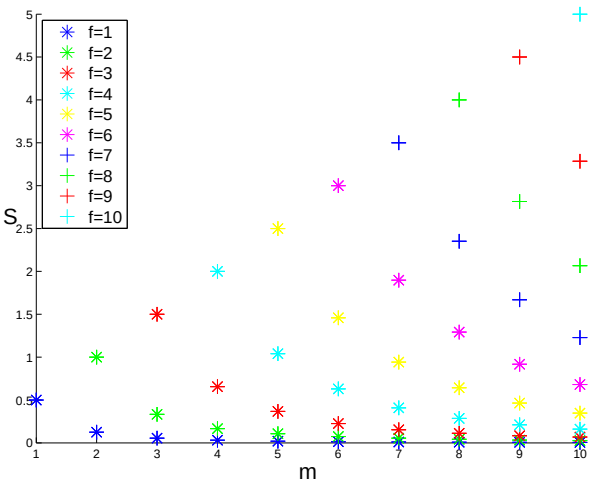



Figure 4.1: The minimal action for up to 10 particles and 10 space-time points.

Good results were obtained with

$$\mu_0 = 1000, \quad \tau_0 = 10^{-10}, \quad \rho = 1.2, \quad \gamma = 0.4, \quad \lambda_0 = 0.$$

The program stops if the local minimizer of the augmented Lagrangian satisfies the restrictions in the accuracy of calculations, i.e. $\sum_{i,j} r_{i,j}(\xi)^2 < 10^{-20}$.
Besides the augmented Lagrangian method, we additionally solve the optimization problem using the interior point algorithm implemented in matlab in order to rule out structural errors which might occur relying on only one numerical solver and in order to double-check the result.

The results are shown in Figure 4.1 and collected in Appendix B. One observes:

- For few space-time points, all local correlation matrices are singular. This implies: The causal structure is in all cases trivial because all points $x, y$ are timelike or lightlike separated.
- If the $F_x$ are singular, in most cases the matrices coincide in its non-trivial eigenvalue, $\mathrm{Tr}(F_x) = \frac{f}{m}$ for all $x \in M$.
- In the case $m = f + 1$, it is $\mathrm{Tr}(A_{xy}) = \frac{1}{m^2}$, and thus the action is given by

$$\mathcal{S}_{\min} = \frac{f\,(1+f^3)}{2(1+f)^3}. \tag{4.2.10}$$

In the following chapter, we will restrict to variational principles on correlation matrices of rank one since these are solutions in special cases. We will discuss the results we have obtained for the general variational principle on fermionic projectors in detail in Section 4.4

## 4.3 The Variational Principle Restricted to Correlation Matrices of Rank One

As the numerics suggest, a global minimizer for only few space-time points yields closed chains $A_{xy}$ of rank one. Since all discrete kernels $P(x,y)$ and thus all local correlation matrices $F_x$ are singular, we can assume that

$$\Psi = \Phi \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \text{for} \quad \Phi \in \text{Mat}(m \times f, \mathbb{C}). \tag{4.3.11}$$

The condition $\Psi^* \Psi = -\mathbb{1}_f$ implies that the columns of $\Phi$ are orthonormal with regard to the standard euclidean scalar product,

$$\Phi^\dagger \Phi = \mathbb{1}_f. \tag{4.3.12}$$

Thus $\Phi$ is an element of the Stiefel manifold $V_f(\mathbb{C}^m)$. The corresponding fermionic projector defined via (2.3.25) is given by

$$P = Q \otimes \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{with} \quad Q = \Phi \Phi^\dagger.$$

The matrix $Q \in \text{Mat}(m \times m, \mathbb{C})$ is hermitian and idempotent with $\text{Tr}(Q) = f$. Denoting for $x \in M$ the vector $u_x = \Phi^\dagger e_x \in \mathbb{C}^f$ as the $x$-th column of $\Phi^\dagger$, the matrix $Q = (q_{xy})$ is the Gramian of $u_1, \ldots, u_m$. According to Definition 2.22, the local correlation matrices corresponding to $P$ are given by

$$F_x = |u_x)(u_x|. \tag{4.3.13}$$

Using that $\text{Tr}\Big((F_x F_y)^2\Big) = \text{Tr}(F_x F_y)^2 = |(u_x|u_y)|^4$, the Lagrangian can be rewritten as

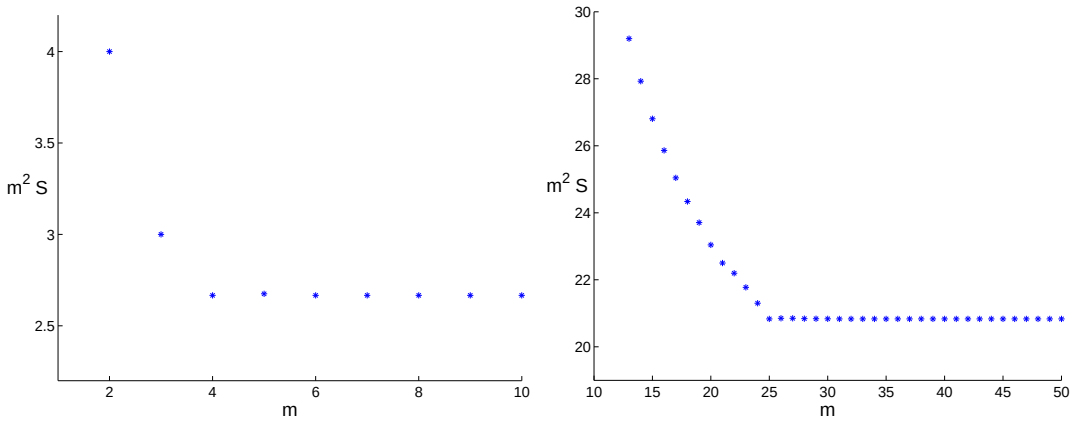
$$\mathcal{L}[F_x, F_y] = \frac{1}{2} |(u_x|u_y)|^4 = \frac{1}{2} |q_{xy}|^4 = \frac{1}{2} \Big| \sum_{k=1}^{f} \Phi_{xk} \overline{\Phi}_{jy} \Big|. \tag{4.3.14}$$

This yields the simplified variational principle

$$\text{minimize} \quad \mathcal{S}[\Phi] = \frac{1}{2} \sum_{x,y=1}^{m} \Big| \sum_{k=1}^{f} \Phi_{xk} \overline{\Phi}_{yk} \Big|^4 \;\; \text{subject to} \;\; \Phi \in V_f(\mathbb{C}^m). \tag{4.3.15}$$

In this setting, the causal structure is trivial as all points are non-spacelike separated.

The simplified setting is numerically much easier to solve, as the problem gets lower dimensional and the target function is now smooth. Scaling the action with the factor $m^2$, the minimal action tends to finite values for $m \to \infty$, which are collected in Table 4.1.




(a) $f = 2$ (b) $f = 5$

Figure 4.2: Plots of the scaled action for rank-one correlation matrices.

| f | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|
| $\lim_{m\to\infty} m^2 \mathcal{S}_{\min}$ | $2\frac{2}{3}$ | 6.75 | 12.8 | $20\frac{5}{6}$ | 30.8572 |

Table 4.1: The asymptotic values of the scaled action for rank-one correlation matrices.

The behavior of the scaled action is exemplary shown in picture 4.2. We note that in all cases equality is approximately attained in the case $m = f^2$. In the case $f = 2$, equality holds for all $m \geq 6$. To see the asymptotic behavior in the case $f \geq 3$, one must consider systems containing more space-time points. In almost all cases, the local correlation matrices have the same trace $\mathrm{Tr}(F_x) = \frac{f}{m}$ for all $x \in M$ and thus yield a family in $\mathcal{F}$, concluding that Corollary 3.17 can be applied. The feature that the scaled action coincides if the number of space-time points is large enough, will be adopted and explained in Chapter 8.

We finally attend to the setting of $m = f + 1$ space-time points, but under the assumption that all local correlation matrices coincide in its traces:

$$\min \; \mathcal{S}[P] \;\; \text{constraint to} \;\; \mathrm{Tr}\big(P(x,x)\big) = \frac{f}{m} \;\; \text{and} \;\; \mathrm{rk}\, P(x,y) \leq 1 \;\; \text{for all} \;\; x, y \in M. \tag{4.3.16}$$

In this special setting, we can prove the following statement:

**Proposition 4.6.** *In the case $m = f + 1$, the minimal action of (4.3.16) is given by*

$$\mathcal{S}_{\min} = \frac{f(1+f^3)}{2(1+f)^3} \tag{4.3.17}$$

*and there exists a minimizer with outer symmetry group $S_m$.*

*Proof.* Let $(F_x)$ denote the family of local correlation matrices corresponding to a fermionic projector satisfying the constraints of (4.3.16), given by

$$F_x = \frac{f}{m} |u_x)(u_x| \quad \text{for} \quad u_x \in \mathbb{C}^f, \quad \|u_x\| = 1.$$

The Cauchy-Schwarz inequality yields for fixed $y \in M$ for the sum of the off-diagonal entries

$$\left( \sum_{\substack{x \in M, \\ x \neq y}} \text{Tr}(F_x F_y) \right)^2 \leq (m-1) \left( \sum_{\substack{x \in M, \\ x \neq y}} \text{Tr}(F_x F_y)^2 \right), \tag{4.3.18}$$

where according to the the identity constraint the right expression is given by

$$\sum_{\substack{x \in M, \\ x \neq y}} \text{Tr}(F_x F_y) = \sum_{x=1}^{m} \text{Tr}(F_x F_y) - \text{Tr}(F_y^2) = \frac{f}{m} - \frac{f^2}{m^2}.$$

Thus the action can be estimated as

$$2\,\mathcal{S}[P] = \sum_{y \in M} \left( \sum_{x \neq y} \text{Tr}(F_x F_y)^2 \right) + \sum_x \text{Tr}(F_x^2)^2 \geq \frac{f^2(m - 2f + f^2)}{m^2(m-1)}.$$

Equality in (4.3.18) holds if and only if the traces $\text{Tr}(F_x F_y)$ for all $x \neq y$ coincide or, equivalently, the vectors $(u_x)$ satisfy

$$|(u_x|u_y)| = \frac{1}{f} \quad \text{for all} \quad x \neq y.$$

We define the matrix $G \in \text{Mat}(m \times m, \mathbb{C})$ as

$$g_{xx} = 1 \text{ for } x \in M \text{ and } g_{xy} = -\frac{1}{f} \text{ for all } x \neq y.$$

The matrix $G$ is diagonally dominant and thus positive semi-definite. The vector $v = -e_1 + \sum_{x=2}^{m} e_x \in \mathbb{C}^m$ (where $e_x$ denotes the $x$-th unit vector in $\mathbb{C}^m$) satisfies $v^\dagger G v = 0$, concluding that $G$ is singular. Since the leading principal submatrix of $G$ of size $m \times m$ is strictly diagonally dominant and thus positive definite, it is $\text{rk}\, G = f$. According to Proposition 3.12, there exist vectors $u_1, \ldots u_{f+1} \in \mathbb{C}^f$ such that the corresponding Gramian coincides with $G$. The fermionic projector corresponding to the local correlation matrices $F_x = \frac{f}{m} |u_x)(u_x|$ solves (4.3.16), where the discrete kernels are calculated as

$$P(x,y) = (u_x|u_y) \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

With regard to Definition 2.12, we conclude that the fermionic projector has outer symmetry group $S_m$. □

Under the additional assumptions of (4.3.16), justified by the numerical solutions, we have completed the symmetry considerations of Theorem 2.13.

## 4.4 The Spontaneous Generation of a Causal Structure

The simplified setting can be used to refine and compare the solutions of the original problem as the optimization task is easier to solve. If the number of space-time points gets large, this minimizer yields only a local but no global minimum. In order to analyze the causal structure, we will plot the matrix $(\mathcal{D}[F_x, F_y])_{x,y \in M}$ and color the entries according to the temperature scheme. Thus positive values are red, zero entries are white and negative values are blue colored.

### 4.4.1 Discrete Fermion Systems of Two Particles

We begin to analyze the numerical results in a discrete fermion system of two particles, and render the results already worked out in [5] for less than 9 space-time points. These systems are most convenient, as we can illustrate the local correlation matrices according to Section 3.1 with a family $(\vec{c}_x)_{x \in M}$ of Bloch vectors.

$m = 2$: We can apply Proposition 4.3. The Bloch vectors lie on a line, $\vec{c}_2 = -\vec{c}_1$.

$m = 3$: The minimizing fermionic system is permutation symmetric, distinct points are timelike separated. The Bloch vectors build a plane equilateral triangle and are unique up to rotations.

$m = 4$: There cannot exist a discrete fermion system with outer symmetry group $S_4$. The Bloch vectors form a tetrahedron which is either left or right oriented. This chirality reduces the outer symmetry group to the group $A_4$, the alternating group of even permutations, which preserve the orientation.

$m = 5$: Now the translation symmetry is broken. The local traces no longer coincide, consequently the fermionic projector is not homogeneous. In particular, it is $\mathrm{Tr}(F_x) \approx 0.388388$ for three space-time points and $\mathrm{Tr}(F_x) \approx 0.407741$ for two space-time points. Thus the Bloch vectors have different lengths, the two shorter vectors lie on a straight line, whereas the other three vectors build an equilateral triangle in the plane orthogonal to the two vectors, see Figure 4.3. The symmetry group is $S^3$. There exist exactly one pair $x \neq y$ which is lightlike separated, all other points are timelike separated.

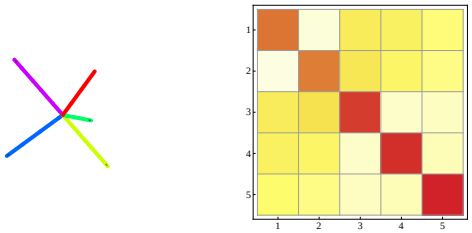



Figure 4.3: Bloch vectors and plot of the matrix $\mathcal{D}$ in the case $m = 5$, $f = 2$.

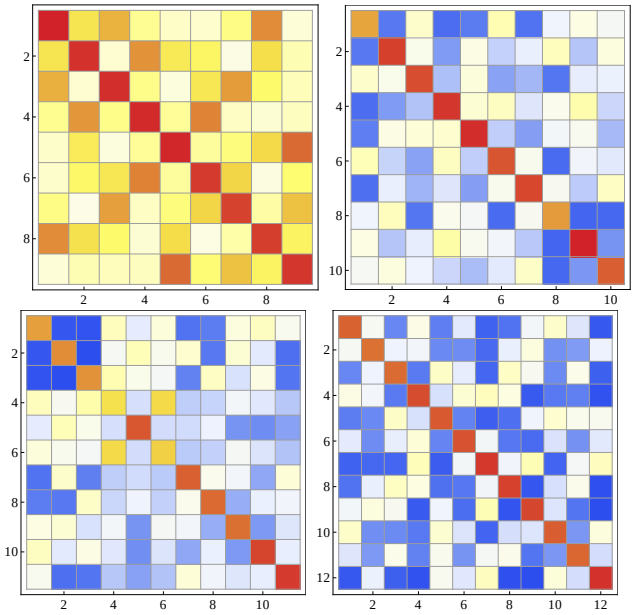


Figure 4.4: Plots of the matrix $\mathcal{D}$ for $f = 2$ and $9 \leq m \leq 12$ (left to right, up to down).

$6 \leq m \leq 9$: All local correlation matrices $F_x$ are singular and have the same non-vanishing eigenvalue $f/m$. There exist many different minimizers. All points are lightlike or timelike separated.

$m = 10$: For the first time, the minimizer of the simplified setting (4.3.15) yields an action which is strictly larger than the action of the original variational principle (4.2.7). We found

$$\inf \mathcal{S}[\Phi] = 0.026666\ldots > \inf \mathcal{S}[\Psi] = 0.0257538\ldots.$$

The local correlation matrices $F_x$ are now rank-two matrices, which no longer coincide in its spectra. The causal structure changes, there exist points which are spacelike separated, as can be seen in Figure 4.4. The fermionic projector whose fermion matrix is given by (4.3.11) is only a local minimum.

$m = 11$: Again the local correlation matrices are rank-two matrices and

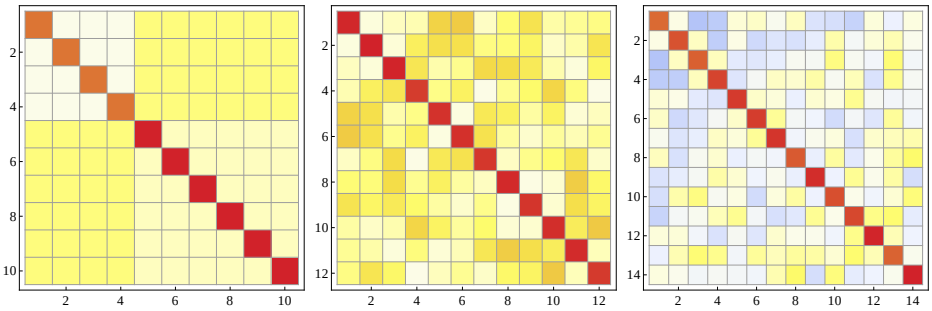
$$\inf \mathcal{S}[\Phi] = 0.0220386\ldots > \inf \mathcal{S}[\Psi] = 0.0213274\ldots.$$

The causal structure is non-trivial, there exist points which are timelike/lightlike/spacelike separated.

$m = 12$: Again the local correlation matrices are rank-two matrices and

$$\inf \mathcal{S}[\Phi] = 0.0185185\ldots > \inf \mathcal{S}[\Psi] = 0.0167513\ldots.$$

The local correlation matrices approximately coincide in its two non-trivial eigenvalues.



(a) $m = 10$ (b) $m = 12$ (c) $m = 14$

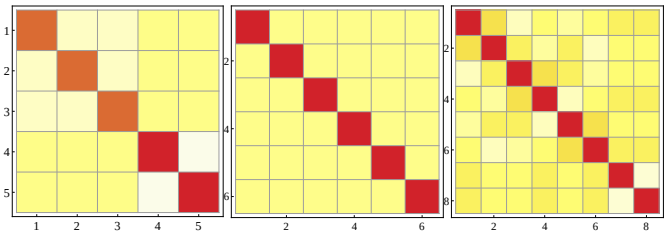
Figure 4.6: Plots of the matrix $\mathcal{D}$ for $f = 3$ and larger $m$.

### 4.4.2 Discrete Fermion Systems of Three Particles

In the case $f \geq 3$, we can only illustrate the system with Lorentz vectors in the Minkowski space according to Section 3.2.2 if the family of local correlation matrices lies in $\mathcal{F}$. We skip the case $f = m$, and treat the case $m = f + 1$ just shortly, since in all cases Proposition 4.6 can be applied. In the case $m > f + 1$, it is difficult to determine the outer symmetry group, the pictures of the matrices $\mathcal{D}[F_x, F_y]$ can be used for suggesting the symmetry.

$m = 4$: The minimizing discrete fermion system has $S_4$-symmetry.

$m = 5$: Again the translation symmetry is broken. The local traces no longer coincide, as it is $\mathrm{Tr}(F_x) \approx 0.596862$ three times, $\mathrm{Tr}(F_x) \approx 0.604708$ twice. All points are lightlike or timelike separated. The causal structure looks similar to the case of two particles, as can be seen in Figure 4.5



(a) $m = 5$ (b) $m = 6$ (c) $m = 8$

Figure 4.5: Plots of the matrix $\mathcal{D}$ for $f = 3$ and small $m$.

$6 \leq m \leq 9$: The local correlation matrices are all singular and coincide in its trace. In the case $m = 6, 7, 9$ the traces $\mathrm{Tr}(F_x F_y)$ for all $x \neq y$ are equal, see Figure 4.5

$m = 10$: The local traces do not coincide because it is $\mathrm{Tr}(F_x) \approx 0.296204$ four times, 0.302531 six times, indicating that the outer symmetry group is reduced to a smaller group.

$11 \leq m \leq 13$: The local traces of the singular matrices $F_x$ are all different, but in a small interval.

$m = 14$ : For the first time we observe that the solution of the simplified principle is not the solution of the variational principle as it is

$$\inf \mathcal{S}[\Phi] = 0.0344388\ldots > \inf \mathcal{S}[\Psi] = 0.034426\ldots.$$

All local correlation matrices are rank-two matrices with non-trivial eigenvalues which do not coincide. With regard to Figure 4.6, there exist points which are spacelike, timelike and lightlike separated.

$m = 15$: Again we observe a non-trivial causal structure with

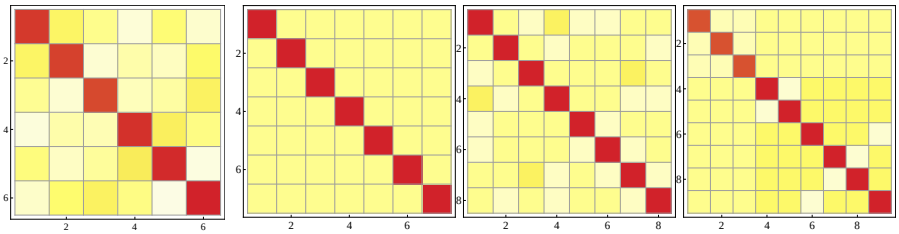
$$\inf \mathcal{S}[\Phi] = 0.03 > \inf \mathcal{S}[\Psi] = 0.029343\ldots.$$

### 4.4.3 Discrete Fermion Systems of Four Particles

The situation in the case $f = 4$ and few space-time points is similar, see Figure 4.7:

$4 \leq m \leq 8$: All local correlation matrices are singular with $\mathrm{Tr}(F_x) = \frac{f}{m}$ for $x \in M$.

$m = 9$: The local traces no longer coincide, as it is $\mathrm{Tr}(F_x) \approx 0.441898$ for three, $\mathrm{Tr}(F_x) \approx 0.445718$ for six points. All points are lightlike or timelike separated. The causal structure looks quite similar as in the case of two particles.



(a) $m = 6$ (b) $m = 7$ (c) $m = 8$ (d) $m = 9$

Figure 4.7: Plots of the matrix $\mathcal{D}$ for $f = 4$.

We expect a change of the causal structure in the case of four and more particles like we have observed for two and three particles, but the numerics did not yield a minimizer with spacelike separated points for four particles and less than 16 space-time points. It does not seem reasonable to consider higher systems with the used numerical solvers because the procedures get very slow and many local minima appear.

To sum the results up, the variational principle favors in special cases the fermionic projector which implies symmetric structures. If the system is sufficiently large, the fermionic projector causes a change of the causal structure, there occur points which are spacelike separated. In order to understand these occurrences, we will now analyze the variational principle restricted to the homogeneous setting.

# 5 Causal Variational Principles on the Sphere

## 5.1 Analysis of the Variational Principles

From now on, we investigate the variational principle in matrix formulation (2.2.18) restricted on hermitian matrices which satisfy the properties (E) and (F2). In regard of the previous chapter, we minimize the rescaled action

$$\mathcal{S}[(F_x)] = \frac{1}{m^2} \sum_{x,y=1}^{m} \mathcal{L}\,[F_x, F_x] \tag{5.1.1}$$

by varying $(F_x)_{x \in M}$ in the family $\mathcal{F}$ of hermitian $f \times f$ with prescribed simple eigenvalues $\alpha, -\beta$. In this case, the diagonal entries of the Lagrangian are calculated as

$$\mathcal{L}[F_x, F_x] = \frac{1}{2}(\alpha^2 - \beta^2)^2. \tag{5.1.2}$$

Consequently, the estimate (4.1.3) yields

$$\mathcal{S}[(F_x)] \geq \frac{1}{m^2} \sum_{x=1}^{m} \mathcal{L}\,[F_x, F_x] = \frac{1}{2m}(\alpha^2 - \beta^2)^2. \tag{5.1.3}$$

We start our analysis with the case of two particles. These systems are special as we can identify each matrix in $\mathcal{F} \subset \mathrm{Mat}(2 \times 2, \mathbb{C})$ with a vector on the sphere. Additionally, we can construct the Gramian easily by noticing that the Stiefel manifold is $V_2(\mathbb{C}^2) = \mathrm{U}(2)$. We start with few remarks on the Gramian, introduced and constructed in Section 3.2.2. By applying Propositions 3.11 and 3.12, we obtain

**Corollary 5.1.** *Let $G \in \mathrm{Mat}(2m \times 2m, \mathbb{C})$ be partitioned as in (3.2.17), where $G_{xx} = \mathbb{1}_2$ for all $x \in M$. Then $G$ is positive semi-definite with $\mathrm{rk}(G) = 2$ if and only if*

$$G_{xy} \in \mathrm{U}(2) \quad \text{and} \quad G_{xy} G_{yz} = G_{xz} \quad \text{for all} \quad x < y < z. \tag{5.1.4}$$

Constructing the Gramian $G$ of rank two, we choose $W_1 = \mathbb{1}_2$ and $W_x \in \mathrm{U}(2)$ for $x = 2, \ldots, m$ and define $G$ via (3.2.19). According to (3.2.24), without loss of generality one may choose $W_x \in \mathrm{SU}(2)$, which can be written as

$$W_x = U(r_x, \varphi_x, \psi_x) = \begin{pmatrix} r_x\, e^{i\varphi_x} & R_x\, e^{i\psi_x} \\ -R_x e^{-i\psi_x} & r_x\, e^{-i\varphi_x} \end{pmatrix} \tag{5.1.5}$$

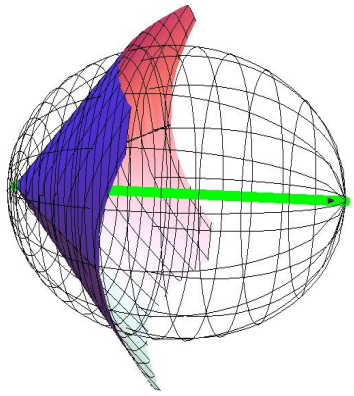


Figure 5.1: The causal structure for space-time points $y$ relative to the base point $x$ in the case $\alpha = 1.8$ and $\beta = 0.2$.

for $R_x = \sqrt{1 - r_x^2}$, $\varphi_x, \psi_x \in [0, 2\pi)$ and $0 \leq r_x, R_x \leq 1$. Consequently, the part $G_{xy}$ of the Gramian $G$ is given by $G_{xy} = W_x^\dagger W_y =: U(r_{xy}, \varphi_{xy}, \psi_{xy})$ with

$$r_{xy}^2 = r_x^2\, r_y^2 + R_x^2\, R_y^2 + 2\, r_x\, r_y\, R_x\, R_y\, \cos(\underbrace{-\varphi_x + \varphi_y - \psi_x + \psi_y}_{=\vartheta_{xy}}). \tag{5.1.6}$$

According to (3.2.23), for $x, y \in M$ the Lorentz vector is

$$\vec{v}_{xy} = \begin{pmatrix} \frac{1}{2}(\alpha^2 - \beta^2)\, r_{xy}^2 \\ \sqrt{\alpha\beta}(\alpha + \beta)\, r_{xy}\, R_{xy}\, \sin(\varphi_{xy} + \psi_{xy}) \\ \sqrt{\alpha\beta}(\alpha + \beta)\, r_{xy}\, R_{xy}\, \cos(\varphi_{xy} + \psi_{xy}) \end{pmatrix}. \tag{5.1.7}$$

The Minkowski norm of this vector and thus the function $\mathcal{D}[L_{xy}]$ is calculated as

$$\mathcal{D}[L_{xy}] = 2\langle\langle \vec{v}_{xy}, \vec{v}_{xy} \rangle\rangle = \frac{1}{2}(\alpha + \beta)^2\, r_{xy}^2 \Big( (\alpha + \beta)^2\, r_{xy}^2 - 4\, \alpha\beta \Big). \tag{5.1.8}$$

Consequently, the causal structure depends only on $r_{xy}$:

$$\begin{aligned} &\text{if } r_{xy}^2 > \tfrac{4\alpha\beta}{(\alpha+\beta)^2} \text{ then } x, y \text{ are timelike separated,} \\ &\text{if } r_{xy}^2 = \tfrac{4\alpha\beta}{(\alpha+\beta)^2} \text{ then } x, y \text{ are lightlike separated,} \\ &\text{if } r_{xy}^2 < \tfrac{4\alpha\beta}{(\alpha+\beta)^2} \text{ then } x, y \text{ are spacelike separated.} \end{aligned}$$

We set $\chi = \varphi_{xy} + \psi_{xy}$ and use the general formula for an ellipsoid centered on the origin, given by $\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} = 1$. Varying $r$ and $\chi$, the family of Lorentz vectors $\vec{v}$ describes an ellipsoid centered at $M = \frac{1}{4}(\alpha^2 - \beta^2)e_0$ with radii $a = \frac{1}{4}(\alpha^2 - \beta^2)$, $b = c = \frac{1}{2}\sqrt{\alpha\beta}(\alpha + \beta)$. This can exemplarily be seen in Figure 5.1, where the vector $\vec{v}_{xx}$ (green) together with the ellipsoid described by the family of vectors $\vec{v}_{xy}$ for $r \in [0, 1]$ and $\chi \in [0, 2\pi]$ and the light-cone are shown.

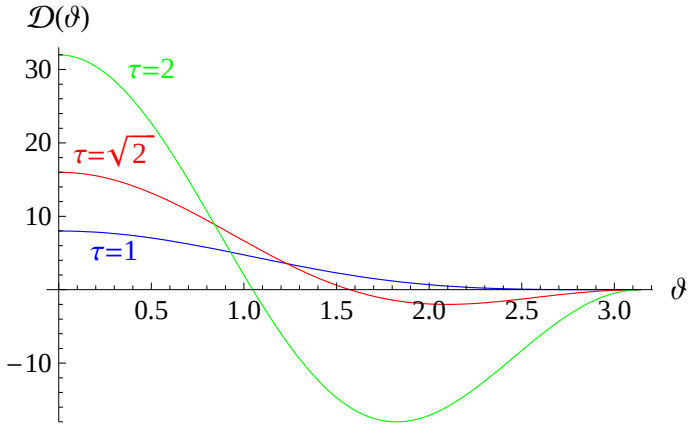



Figure 5.2: The function $\mathcal{D}$.

Additionally, we adopt the approach of Section 3.1. According to Corollary 3.3, each matrix in $\mathcal{F}$ can be identified with a Bloch vector on the sphere. If $\alpha$ and $-\beta$ denote the non-trivial eigenvalues, each matrix in $\mathcal{F}$ can be written as

$$\rho\, \mathbb{1} + r\, x \cdot \vec{\sigma} \quad \text{where} \quad x \in S^2, \quad \rho = \frac{\alpha - \beta}{2},\ r = \frac{\alpha + \beta}{2}.$$

The function $\mathcal{D}$ in (3.1.9) and thus the Lagrangian as the positive part of $\mathcal{D}$ simplify to a function on the sphere,

$$\mathcal{D} : S^2 \times S^2 \to \mathbb{R}, \quad \mathcal{D}(x,y) = 2\,\rho^2\, r^2 + 2\,\rho^2\, r^2\ (x \cdot y) - r^4 \left(1 - (x \cdot y)^2\right),$$

where $\cdot$ denotes the standard dot product on $\mathbb{R}^3$. We parametrize the eigenvalues as

$$\alpha = 1 + \tau, \quad \beta = \tau - 1 \quad \text{for} \quad \tau \geq 1. \tag{5.1.9}$$

As in this case $r = \tau$ and $\rho = 1$, the function $\mathcal{D} : S^2 \times S^2 \to \mathbb{R}$ is given by

$$\mathcal{D}(x,y) = 2\tau^2\, (1 + x \cdot y)\left(2 - \tau^2\, (1 - x \cdot y)\right). \tag{5.1.10}$$

The function depends only on the angle $\vartheta_{xy}$ between the points $x, y \in S^2$ defined by $\cos\vartheta_{xy} = x \cdot y$. Considered as function of $\vartheta \in [0, \pi]$, $\mathcal{D}$ has its maximum at $\vartheta = 0$ and is minimal if $\cos(\vartheta) = -\tau^{-2}$. Moreover, $\mathcal{D}(\pi) = 0$. Typical plots are shown in Figure 5.2. In the case $\tau > 1$, the function $\mathcal{D}$ has two zeros at $\pi$ and

$$\vartheta_{\max} := \arccos\left(1 - \frac{2}{\tau^2}\right). \tag{5.1.11}$$

In view of (2.4.30), the Lagrangian is positive if and only if $0 \leq \vartheta < \vartheta_{\max}$. Thus $\mathcal{I}(x)$ is an open spherical cap, and $\mathcal{J}(x)$ is its closure together with the antipodal point of $x$,

$$\mathcal{I}(x) = \{y \ :\ x \cdot y > 1 - \frac{2}{\tau^2}\}, \qquad \mathcal{J}(x) = \overline{\mathcal{I}(x)} \cup \{-x\}$$

If $\tau$ increases, the opening angle $\vartheta_{\max}$ of the light-cones gets smaller. In the degenerate case $\tau = 1$, the function $\mathcal{D}$ is decreasing, non-negative and has exactly one zero

at $\vartheta = \pi$. Hence the Lagrangian $\mathcal{L}$ coincides with $\mathcal{D}$, all points on the sphere are timelike separated except for antipodal points. The light-cones are $\mathcal{I}(x) = S^2 \backslash \{-x\}$ and $\mathcal{J}(x) = S^2$. If $\tau$ is sufficiently large, the opening angle of the light-cones is so small that the $m$ points can be distributed on the sphere such that any two different points are spacelike separated. In this case, the action becomes

$$\mathcal{S} = \frac{1}{m}\, \mathcal{L}(\vartheta = 0)\,,$$

and in view of (5.1.3) minimal. The question, for which $\tau$ such a configuration exists, leads us to the *Tammes problem*.

## 5.2 The Relation to the Problem of Tammes

The *problem of Tammes* resp. *best packing problem on the sphere* asks for an arrangement of $m$ points on the sphere such that the minimal spherical distance between distinct points is maximized, see [23]:

$$x_1, \ldots, x_m \in S^2 \quad \text{such that} \quad \min_{1 \le i < j \le m} \arccos(x_i \cdot x_j) \quad \text{is maximal.} \tag{5.2.12}$$

Equivalently one can ask for the maximal radius $r$ such that $m$ spherical caps of radius $r$ do not overlap. The set $X_m = \{x_1, \ldots, x_m\} \subset S^2$ of $m$ points on the sphere is called *spherical code*. Due to compactness, a spherical code $X_m$ that solves (5.2.12) exists.

Until now, the Tammes problem is only solved explicitly if $m \le 12$ and for $m = 24$ (for details see [4] and the references therein). For special values of $m$, the solutions of the Tammes problem are symmetric solids like the tetrahedron ($m = 4$), the octahedron ($m = 6$), the icosahedron ($m = 12$) and the snub cube ($m = 24$). Moreover, much research has been done on the numerical evaluation of spherical codes, mostly by N.J.A. Sloane, with the collaboration of R.H. Hardin, W.D. Smith and others, [28], containing numerical solutions of the Tammes problem for up to 130 points.

The Tammes problem is related to the variational principle on the sphere as follows: Let $\vartheta_m$ denote the maximal angle between the points of the spherical code that solves the Tammes problem,

$$\vartheta_m = \max_{x_1, \ldots, x_m \in S^2} \min_{i \neq j} \arccos(x_i \cdot x_j)\,.$$

The optimal spherical code minimizes the action (5.1.1) if the optimal angle $\vartheta_m$ of the Tammes problem is equal to or less than the critical angle $\vartheta_{\text{max}}$ given by (5.1.11). Thus the value of $\tau$ from which on all distinct points in a spherical code of $m$ points can be separated spacelike can be calculated as

$$\tau_m = \sqrt{\frac{2}{1 - \cos(\vartheta_m)}}. \tag{5.2.13}$$

If $\tau \geq \tau_m$, the solution of the Tammes problem is a solution of the variational principle for $m$ points, as the lower bound (5.1.3) of the action is attained. In the case $\tau = \tau_m$, the solutions of the variational principle are exactly the spherical codes $X_m$ that solve (5.2.12). In the case $\tau > \tau_m$, the open light-cones $\mathcal{I}(x)$ decrease, thus a slight distortion of the optimal spherical code $X_m$ does not change the action, concluding that there exist infinitely many different minimizers. In the case $\tau < \tau_m$, there has to be at least one pair of distinct points which contributes to the action, thus the estimate (5.1.3) is strict.

Besides calculations of explicit solutions, efforts have been made to estimate the maximal spherical distance $\vartheta_m$. Using an estimate by W. Habicht and B.L. van der Waerden for the solution $\vartheta_m$ (see [23, page 6]), we obtain an estimate for the value $\tau_m$ given by (5.2.13),

$$4 \left( \left( \frac{8\pi}{\sqrt{3}m} \right)^{1/2} - \frac{C}{m^{2/3}} \right)^{-2} \;\geq\; \tau_m^2 \geq 4\, \frac{\sqrt{3}m}{8\pi} \tag{5.2.14}$$

for some constant $C > 0$.

## 5.3 Global Optimization using Simulated Annealing

We now solve the action principle on the sphere numerically. Using spherical coordinates, each vector in $S^2$ can be written as

$$v(\vartheta, \varphi) := \begin{pmatrix} \sin(\vartheta)\cos(\varphi) \\ \sin(\vartheta)\sin(\varphi) \\ \cos(\vartheta) \end{pmatrix}, \tag{5.3.15}$$

where $\vartheta \in [0, \pi]$ and $\varphi \in [0, 2\pi)$. In the numerical approach, we allow both angles to obtain arbitrary values, loosing the uniqueness but gaining an unconstrained minimization problem on $\mathbb{R}^{2m}$. According to (5.1.2) and the symmetry of the Lagrangians, instead of minimizing $\mathcal{S}$ we can restrict on minimizing

$$\hat{\mathcal{S}} = \frac{1}{m^2} \sum_{i<j} \mathcal{L}(x_i, x_j).$$

The need of a global optimization routine can be illustrated by considering the dependence of the target function on the variables. This is done in Figure 5.3 by taking the spherical code $X_{20}$ that solves the Tammes problem and plotting for different values of $\tau$ the action $\mathcal{S}$ considered as a function of only $\vartheta_1$, where $x_1 = v(\vartheta_1, \varphi_1)$. Many local minima appear and reveal that attempts using a local minimization routine may not yield satisfying results. The plots in Figure 5.3 also show that the structural behavior of the action changes. In the case $\tau = 1$, the target function is smooth and there only exists one global minimum for each variable. In

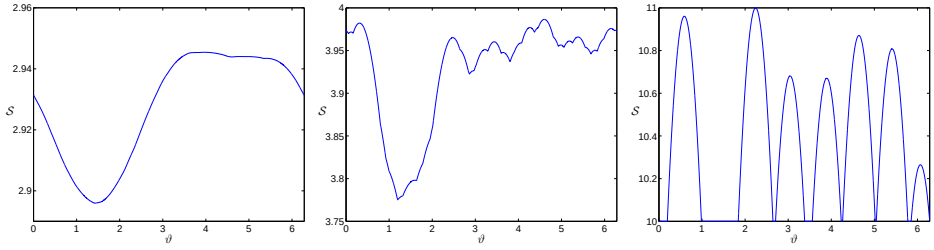


Figure 5.3: The action depending on $\vartheta_1$ for $\tau = 1.3$ (left), $\tau = 2$ (middle) and $\tau = 5$ (right).

this case, the matrices $F_x$ are rank-one matrices, and this observation justifies the use of a local routine to solve the problems in chapter 3. If $\tau > 1$, the target function gets non-smooth with many local minima. For $\tau$ close to one, there exist only few local minima, which are not very pronounced, so that even a local minimization routine may find satisfying solutions. For $\tau \gg 1$, the situation again gets more easy, as there is only one pronounced minimal value. In the remaining interval, the target function is non-smooth with many points of discontinuity and many local minima.

In order to solve the minimization problem, we need a global optimization method which allows to take a direction yielding higher function values in order to escape a local minimum and attain a branch leading to the global minimum, and which does not require differentiability. A common routine is the method of *simulated annealing*, (see [6] and the references therein), which is a probabilistic metaheuristic algorithm based on annealing in metallurgy. Heating a material gives atoms the freedom to move and randomly distribute. Cooling the material again down slowly, the atoms arrange themselves in a ground state of minimal energy state. In the process, the atoms escape an energy state which is locally minimal by shortly accepting a higher energy state. The simulated annealing algorithm adopts this process to find the global minimum of a function $f : D \subseteq \mathbb{R}^n \to \mathbb{R}$. The basic steps of the algorithm starting at the vector $x \in D$ are

a) local change: choose vector $y$ close to $x$,

b) selection: if $f(y) \leq f(x)$ then $y \leftarrow x$, else $y \leftarrow x$ with probability $e^{-\frac{f(y)-f(x)}{T}}$.

A vector is accepted despite a higher function value with a probability determined by the temperature $T$. To achieve a local minimum, the temperature decreases and converges to 0, thus a point with a lower function value is accepted less probably in the process. The local change of the vector is realized by a mapping $U : D \to D$, which maps $x \in D$ at a vector $y$ close to $x$. For example, one can perturb one randomly chosen entry of $x$, thus $y_k = x_k + r$ for random numbers $k, r$, and $y_i = x_i$ else. To decrease the temperature on the run, one needs the cooling schedule $C : \mathbb{R}^+ \to \mathbb{R}^+$, which is a monotone decreasing function with $\lim_{n\to\infty} C^n(T) = 0$, where we use the geometric cooling scheme $C(T) = a^T$ for $a \in (0, 1)$.
The process stops, if either the temperature gets too small or a loop is run too often without changing the solution vector and thus stays in a local minimum. The algorithm uses the following parameters:

- $c$ counts the number of passes the solution vector stays unchanged. If a vector with a lower function value is found, the value of $c$ is again set 0 . If $c > c_{\max}$, the algorithm stops.
- $i$ counts the number of iterations done with one fixed temperature. If $i$ gets too large, the temperature is decreased and $i$ is reset 1.
- $s$ counts, how often the solution vector with a fixed temperature gets changed. If $s$ gets too large, the temperature gets decreased and $s$ is reset 1.
- *rand* is a random number in $[0, 1]$ and determines, if the new vector is accepted despite a higher function value. This number gets regenerated in each step.
- $\tau$: the new vector $y$ is accepted despite a higher function values if this value differs from the old function value at less than $\tau$.

This leads to the

**Algorithm 5.2.** *Simulated annealing*

***Start*** $x \in D$, $i = 1$ , $c = 0$, $s = 1$, $T > 0$
***while*** $c < c_{max}$ *and* $T > T_{min}$ ***do***
  $i \leftarrow i + 1$
  ***if*** $i > i_{max}$ $||s > s_{max}$ ***then***
    $T = C(T)$, $i = 1$, $s = 1$
  ***end if***
  $y = U(x)$
  ***if*** $f(x) - f(y) > \tau$ ***then***
    $y \leftarrow x$, $s \leftarrow s + 1$, $c \leftarrow 0$
  ***else***
    ***if*** *rand* $< \exp\left(\frac{f(x)-f(y)}{T}\right)$ ***then***
      $x \leftarrow y$, $c \leftarrow 0$
    ***else***
      $c \leftarrow c + 1$
    ***end if***
  ***end if***
***end while***

The choice of the initial and the stopping temperature has to be done carefully. The initial temperature determines the acceptance of vectors yielding a higher function value. A low initial temperature will fall into a local minimum, but if the initial temperature is chosen too high, all vectors are accepted. A high stopping temperature yields a lower stopping point but causes longer CPU-time.

We use the general simulated annealing algorithm in [30]. For a discussion of the algorithm, a value of $\tau$ is adequate, such that all distinct points can be separated spacelike and thus we already know the minimal action $\hat{\mathcal{S}} = 0$. We take $m = 20$ and $\tau = 2.5 > \tau_{20}$. Starting with a random spherical code $X$ with $\hat{\mathcal{S}}(X) = 6.167855$

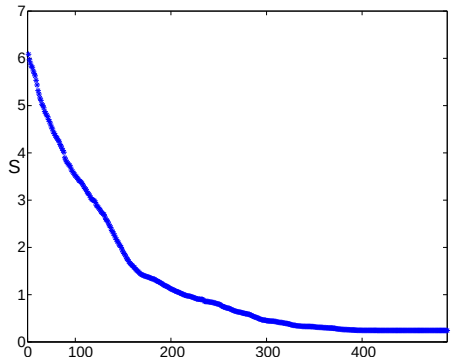



Figure 5.4: The development of the action $\hat{\mathcal{S}}$ in the simulated annealing algorithm.

and using the structural parameters InitTemp= 1, MaxConsRej= 1000, StopTemp= $1.0e-16$, MaxSuccess= 20, CoolSched: $T = 0.8 * T$, MaxTries= 300, the algorithm stops after 15.902203 seconds with $\hat{\mathcal{S}} = 0.241036$. The progress of the function is shown in Figure (5.4).

This result is not deeply satisfying. Additionally, as the simulated annealing yields only randomly good results, the same routine with the same starting vector will yield different results, which may be even higher. To counteract this probabilistic behavior, it is promising to repeat the algorithm, additionally adjusting the parameters. As the most crucial parameter is the temperature, it seems reasonable to start with a high temperature and scale it down in each step, and slowly freezing the system in the global minimum, see Appendix C.

**Algorithm 5.3** (annealing loop). ***Start*** $x \in D$, $T = f(x)$, $b \in (0,1)$
***while*** $T > T_{min}$ ***do***
$y = anneal(f, x)$ *with initial temperature* $T$
$T \leftarrow bT$
***if*** $f(x) > f(y)$ ***then***
$x \leftarrow y$
***end if***
***end while***

Starting this loop, the vectors are free to overcome a local minimum, while with repeating the annealing the minimum gets refined. The development of one loop can be seen in Figure 5.5 left, where the action stopped after 62.797773 seconds with $\hat{S} = 0$ in accuracy of calculation. In practice, this procedure does not always succeed, see Figure 5.5 right, thus may be repeated with higher parameters and other starting vectors.

We are interested in the global minimizer of the variational principle for different values of $\tau$. Since the function $\mathcal{D}$ depends smoothly on $\tau$, the solution obtained for a certain value of $\tau$ contains informations which can be used solving the slightly different problem for a lower or higher value of $\tau$. Thus we proceed as follows, see Appendix C: We apply the loop of simulated annealing for the function at $\tau = 1$, choosing as starting vector the known solution of the Tammes problem $X_m$. For a stepsize $h$, we increase the parameter $\tau$ in each step via $\tau \leftarrow \tau + h$ (we will choose

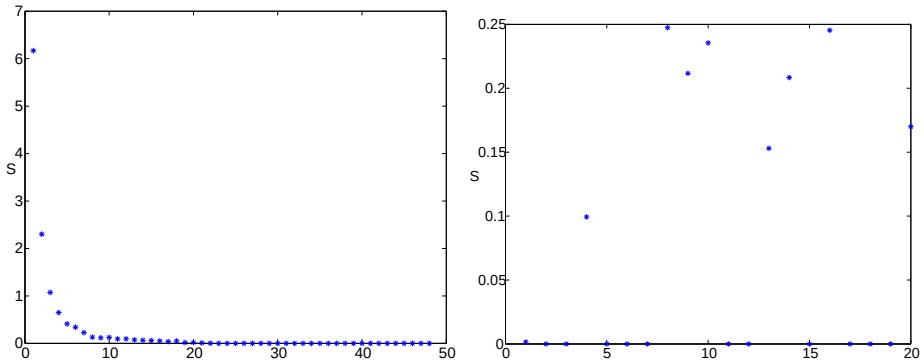



Figure 5.5: The action development repeating the annealing algorithm by slowly decreasing $T$ (left) and the final values repeating this process with the same starting vector several times(right).

$h = 0.01$) and apply the annealing loop, using the solution of the previous step as starting vector for the new optimization task. This may be repeated until the critical value $\tau_m$ is exceeded and thus $X_m$ is a known.

As the annealing algorithm will not yield the optimal solution in all cases, we repeat the procedure backwards starting with $\tau > \tau_m$ and slowly decreasing $\tau$ using higher structural parameters. This proceeding refines the already found low value of the action carrying over the information of the slightly different problem for a higher $\tau$-value. It causes many function calls and a high CPU-time, especially if the number $m$ of space-time points is high, but yields reasonable and satisfying results.

We finally remark that for only a small number of space-time points, a local optimization routine yields acceptable results, thus we can check the simulated annealing procedure. If the number $m$ gets larger, the local routine stays in the only local minimum, and thus is no longer appropriate.

## 5.4 Discussion of Solutions for Small Systems

We now analyze the minimizers of the variational principle on hermitian matrices with prescribed eigenvalues $\alpha, -\beta$. For a small number of space-time points, we will be able to explore special features and even prove the global minimum. Studying the spherical code $X_m = \{x_1, \ldots, x_m\}$ of Bloch vectors, we note that a rotation of the whole system does not change the action, thus we can always assume that $x_1 = e_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$.

### Two Space-Time Points

If there are only two space-time points, we are free to choose $W_2 \in \mathrm{SU}(2)$ and thus $r_2$ such that the two distinct points are non-timelike separated, and the lower bound (5.1.3) is attained. The spherical code that solves the Tammes problem is given by $X_2 = \{e_3, -e_3\}$, where $\mathcal{L}(x_1, x_2) = \mathcal{L}(\pi) = 0$. If $\tau = 1$, this is the unique minimizer. If $\tau > 1$, one can choose $x_2$ such that $x_1 \cdot x_2 \leq \cos(\vartheta_{\max})$.

### Three Space-Time Points

In the case of three particles, the parts $G_{12}$ and $G_{23}$ determine $G_{13}$ according to formula (5.1.4), thus it is no longer possible to separate all distinct points spacelike for all values of $\alpha, \beta$:

**Lemma 5.4.** *In the case $f = 2$ and $m = 3$, the minimal action is given by*

$$\mathcal{S}_{\min} = \begin{cases} \frac{1}{16}(\alpha+\beta)^2(3\alpha-\beta)(\alpha-3\beta) & \text{if } \frac{1}{4} > \frac{4\,\alpha\,\beta}{(\alpha+\beta)^2} \\ \frac{1}{6}(\alpha^2-\beta^2)^2 & \text{if } \frac{1}{4} \leq \frac{4\,\alpha\,\beta}{(\alpha+\beta)^2} \end{cases}$$

*Proof.* We set $c = \sqrt{\frac{4\,\alpha\,\beta}{(\alpha+\beta)^2}}$. Let $W_1 = \mathbb{1}_2$ and $W_2, W_3 \in \mathrm{SU}(2)$ be represented as in (5.1.5), which determine $G_{23}$ according to (5.1.4). With regard to formula (5.1.8), the function $\mathcal{D}(L_{13})$ attains its minimum at $\vartheta_{23} = \pi$, in which case $r_{23}$ given as (5.1.6) simplifies to

$$r_{23}^2 = (r_2 r_3 - R_2 R_3)^2 .$$

Regarding $r_{23}^2$ as a function of $r_2$, the minimal value 0 is attained for $r_2 = \sqrt{1-r_3^2}$. If $r_3 \leq c$ it is $\sqrt{1-r_3^2} \leq c$ if and only if $c \geq \frac{1}{\sqrt{2}}$. In the case $c < \frac{1}{\sqrt{2}}$ the function $r_{23}^2$ is minimal if $r_2, r_3$ are maximal, thus one can choose $r_{23} < c$ if and only if $(2c-1)^2 \leq c^2$ or equivalently $c \geq \frac{1}{2}$. We conclude that the lower bound (5.1.3) can be obtained if and only if $c^2 \geq \frac{1}{4}$.
Let now be $c > \frac{1}{2}$. We start with the case $r_2, r_3 \in [c, 1]$. Then the minimization of $\mathcal{S}$ is equivalent to

$$\min\ r_2^2(r_2^2-c^2) + r_3^2(r_3^2-c^2) + r_{23}^2(r_{23}^2-c^2) \ \text{ for } \ r_{23}^2 = (r_2 r_3 - R_2 R_3)^2,\ r_2, r_3 \in [c, 1].$$

This problem is symmetric in $r_2$ and $r_3$. The partial derivative of the function

$$f(r_2, r_3) = r_2^2(r_2^2-c^2) + r_3^2(r_3^2-c^2) + r_{23}^2(r_{23}^2-c^2)$$

is

$$\frac{\partial f}{\partial r_2} = -\frac{2}{R_2 R_3}\ A(r_2, r_3)\ B(r_2, r_3),$$

where

$$\begin{aligned} A(r_2, r_3) =& 2r_2^2 R_3^2 + 2r_2 r_3 R_2 R_3 - R_3^2, \\ B(r_2, r_3) =& \left(c^2 + 2r_2^2 - 2\right) r_3 + 2\left(1 - 2r_2^2\right) r_3^3 - 2r_2 R_2 R_3 (1 - 2r_3^2). \end{aligned}$$

The function $A$ has exactly one zero at $r_2 = \sqrt{\frac{1-r_3}{2}}$, yielding a local minimum of $f(., r_3)$. The function $B$ is always negative, as the following consideration shows: Using that

$$\frac{\partial B}{\partial r_2} = -\frac{2(1-2r_3^2)}{R_2 R_3}\ A(r_2, r_3),$$

where $A$ changes sign only at $r_2 = \sqrt{\frac{1-r_3}{2}}$, we distinguish the following cases:

$1 - 2r_3^2 < 0$: The function $B$ is maximal at $r = \sqrt{\frac{1-r_3}{2}}$ and thus

$$B(r_2, r_3) \leq B\left(\sqrt{\tfrac{1-r_3}{2}}, r_3\right) = r_3\left(c^2 + 2r_3 - 1\right) - 1 < r_3(c^2 - 1 + \sqrt{2}) < 0$$

$1 - 2r_3^2 > 0$: We have the estimate

$$B(r_2, r_3) \leq \left(c^2 + 2r_3^2 - 2\right) r_3 + 2r_2^2 r_3 \left(1 - 2r_3^2\right) \leq r_3(c^2 - 2r_3^2) < 0.$$

$1 - 2r_3^2 = 0$: In this case it is $B\left(r_2, \frac{1}{\sqrt{2}}\right) = \frac{c^2-1}{\sqrt{2}} < 0$.

We conclude that there is exactly one global minimum of $f$ at $r_2 = r_3 = r_{23} = \frac{1}{2}$ with

$$f\left(\tfrac{1}{2}, \tfrac{1}{2}\right) = \tfrac{3}{16}(1 - 4c^2).$$

It remains to consider the cases $r_2, r_3 \notin [c, 1]$.

$r_2 \geq c$, $r_3 \leq c$: In this case, the function we have to minimize is

$$g(r_2, r_3) = r_2^2(r_2^2 - c^2) + r_{23}^2(r_{23}^2 - c^2),$$

where $r_{23}$ is minimal for $r_3 = c$ maximal. Thus $g$ is minimal for $r_2 = \sqrt{\frac{1-c}{2}}$, yielding

$$g(1/2, c) = \tfrac{1}{2}(1 - c)(1 - c - 2c^2) > \tfrac{3}{16}(1 - 4c^2) \quad \text{for} \quad c \in [0, 1/2).$$

$r_2, r_3 \leq c$: In this case, the target function we have to minimize is

$$h(r_2, r_3) = r_{23}^2(r_{23}^2 - c^2),$$

where $r_{23}$ is minimal for $r_2 = r_3 = c$ maximal, yielding

$$h(c, c) = (1 - 2c^2)(1 - 5c^2 + 2c^4) > \tfrac{3}{16}(1 - 4c^2) \quad \text{for} \quad c \in [0, 1/2).$$

This completes the proof. □

The corresponding spherical code is a planar triangle with

$$x_2 = v\left(\tfrac{2}{3}\pi, 0\right) = \begin{pmatrix} \sqrt{3}/2 \\ 0 \\ -1/2 \end{pmatrix} \quad x_3 = v\left(\tfrac{2}{3}\pi, \pi\right) = \begin{pmatrix} -\sqrt{3}/2 \\ 0 \\ -1/2 \end{pmatrix}.$$

This is also the solution of the Tammes problem. The Lagrangians are given by $\mathcal{L}(x_i, x_j) = \mathcal{L}\left(\frac{\pi}{3}\right)$ for all $i \neq j$, and thus we obtain

$$\tau_3 = \frac{2}{\sqrt{3}} \approx 1.15470.$$

The minimal action can be rewritten as

$$\mathcal{S}_{\min} = \mathcal{S}[X_3] = \frac{1}{3}\mathcal{L}(0) + \frac{2}{3}\mathcal{L}\left(\tfrac{\pi}{3}\right).$$

### Four Space-Time Points

For a larger number of points, the minimization problem on the Gramian gets too difficult to be solved analytically. Thus we restrict in the following on the variational principle on the sphere, where the prescribed eigenvalues are given by (5.1.9), and solve this optimization problem numerically as discussed in Section 5.3. The vectors on the sphere minimizing the action principle build a regular tetrahedron and thus coincide with the solution of the Tammes problem. They are given by

$$x_2 = v\,(\gamma_4, 0)\,, \quad x_3 = v\left(\gamma_4, \tfrac{2\pi}{3}\right) \quad x_4 = v\left(\gamma_4, \tfrac{4\pi}{3}\right)$$

with the tetrahedron angle $\gamma_4 = \arccos(-1/3) \approx 109,5°$. The action can be rewritten as

$$\mathcal{S}_{\min} = \mathcal{S}[X_4] = \frac{1}{4}\mathcal{L}\,(0°) + \frac{5}{8}\mathcal{L}\,(\gamma_4)\,,$$

concluding that $\tau_4 = \sqrt{\frac{3}{2}} \approx 1.22474$. The minimizer again breaks the parity symmetry but there exists one configuration which solves the variational principle for all values of $\tau$. This changes if the number of points is again increased.

### Five Space-Time Points

The solution of the Tammes problem for $m = 5$ is not unique. Optimal configurations can be obtained by taking the two poles and placing three points on the equator such that their angle is at least $\frac{\pi}{2}$, yielding an infinite family of solutions. We conclude that for $\tau = \tau_5 = \sqrt{2}$ there also exists an infinite family of solutions of the variational principle.

The solution of the variational principle for smaller $\tau$ seems to be unique up to rotation, but changes for different values of $\tau$. For $\tau$ close to 1, the optimal spherical code $X_5$, where the three points on the equator are placed equidistant, thus

$$x_2 = -e_3, \quad x_3 = e_1, \quad x_4 = v\left(\frac{\pi}{2}, \frac{2\pi}{3}\right), \quad x_5 = v\left(\frac{\pi}{2}, \frac{4\pi}{3}\right), \tag{5.4.16}$$

minimizes the variational principle with corresponding action

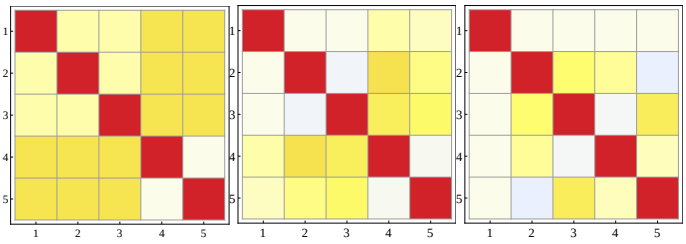
$$\mathcal{S}_{\min} = \mathcal{S}[X_5] = \tfrac{1}{5}\,\mathcal{L}\,(0) + \tfrac{2}{25}\Big(\mathcal{L}\,(\pi) + 6\,\mathcal{L}\,(\pi/2) + 3\,\mathcal{L}\,(2\pi/3)\Big).$$

According to the numerical results, for the first time this point distribution is not a minimizer for $\tau > \tau_3$, in which case $\mathcal{L}\,(2\pi/3) = 0$. In the case $\tau_3 \leq \tau < 1.26$, the causal structure changes, see Figure 5.6, where the points $1, 2$ and $1, 3$ are lightlike separated, the points $2, 3$ and $4, 5$ are spacelike separated. To be more precise, the minimal distribution is given as

$$x_2 = v(\vartheta_{\max}, 0), \quad x_3 = v(\vartheta_{\max}, \pi), \quad x_4 = v(\psi, 0), \quad x_5 = v(\psi, \pi).$$

Assuming these vectors, we can calculate the angle $\psi$ by solving

$$\text{minimize } 2\,\mathcal{L}(x_2, x) + \mathcal{L}(x, -x) \quad \text{for} \quad x = \begin{pmatrix} 0 \\ \sin\psi \\ \cos\psi \end{pmatrix},$$



(a) $\tau = 1$ (b) $\tau = 1.17$ (c) $\tau = 1.27$

Figure 5.6: Plots of the matrix $\mathcal{D}$ for $m = 5$ and $f = 2$.

yielding $\psi = \arccos\left(\frac{4-3\tau^2}{3\tau^4-8\tau^2+8}\right)$, which matches the numerical results. The above points are only a solution if $\psi < \vartheta_{\max}$ or equivalently $\tau < 1.25839$. If $1.26 \leq \tau < \tau_5 = \sqrt{2}$, the structure again changes: There exists one point $x \in M$ with $x \cdot y = \vartheta_{\max}$ for all $y \neq x$. The points $y \neq x$ lie equidistant on the circle of latitude $\{z \in S^2 : x \cdot z = \vartheta_{\max}\}$. The optimal distribution is thus given as

$$x_2 = v(\vartheta_{\max}, 0), x_3 = v(\vartheta_{\max}, \pi/2), x_4 = v(\vartheta_{\max}, \pi), x_5 = v(\vartheta_{\max}, 3\pi/2)$$

with corresponding minimal action

$$\mathcal{S}_{\min} = \frac{1}{5}\, 8\tau^2 + \frac{8}{25}\, \mathcal{L}\left(\arccos(\cos^2 \vartheta_{\max})\right) + \frac{8}{25}\, \mathcal{L}\left(2\vartheta_{\max}\right).$$

As $\mathcal{D}\left(2\vartheta_{\max}\right) < 0$ for all $y \neq x$, there exists exactly one point $z \neq x$ which is spacelike separated from $y$. Thus the variational principle shows a non-trivial causal structure and distinguishes one point apart from the others. The Lorentz vectors $\vec{v}_{xy}$ for $y \in M$ for different base points $x \in M$ no longer coincide, see Figure 5.7.
For five points, concluding, the symmetric structure breaks and the parameter $\tau$ highly affects the structure.

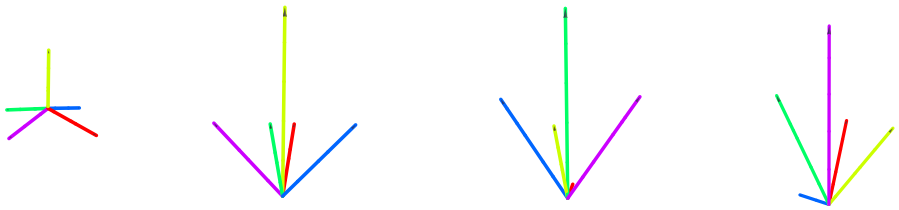


Figure 5.7: The Bloch vectors (left) and the Lorentz vectors relative to the base points 1, 2 and 4 in the case $m = 5$ and $f = 2$ for $\tau = 1.27$.

### Six and more Space-Time Points

**$\mathbf{m = 6}$:** The solution of both the Tammes problem and the variational principle is the octahedron,

$$X_6 = \{\pm e_1, \pm e_2, \pm e_3\}, \tag{5.4.17}$$

concluding that $\tau_6 = \sqrt{2} = \tau_5$. The corresponding action is given by

$$\mathcal{S} = \frac{1}{6}\,\mathcal{L}\,(0) + \frac{2}{26}\,(3\,\mathcal{L}\,(\pi) + 12\,\mathcal{L}\,(\pi/2))\,.$$

**m = 7**: The solution of the Tammes problem does not solve the action principle in the case $\tau = 1$, but there exists a distribution such that $\mathcal{S}_{\min} = 2\frac{2}{3} < \mathcal{S}[X_7]$ for $\tau = 1$. The value of $\tau$ again determines the causal structure: for $\tau$ close to one, all points are timelike separated, whereas for higher values spacelike separated points appear. Increasing $\tau$, one observes that there are no longer seven distinct points, but points coincide and only 6 distinct points appear, concluding that one point is occupied twice.

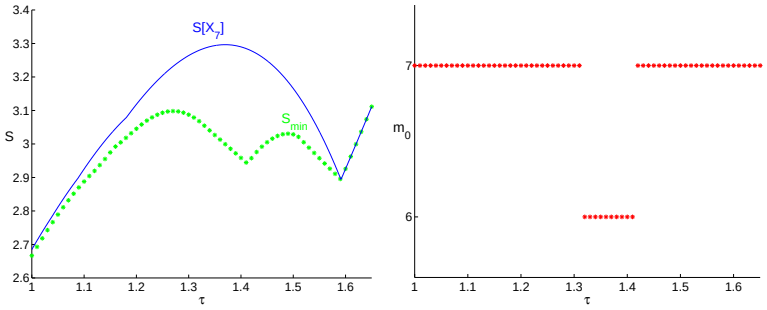



Figure 5.8: The minimal action for 7 points (left) and the number of distinct points(right).

**m = 8**: The solution of the Tammes problem is the square antiprism, denoted by $X_8$. The cube, whose spherical code we denote by $W_8$, solves the variational principle in the case $\tau < \tau_3$. Again increasing $\tau$, there also occur less distinct points.

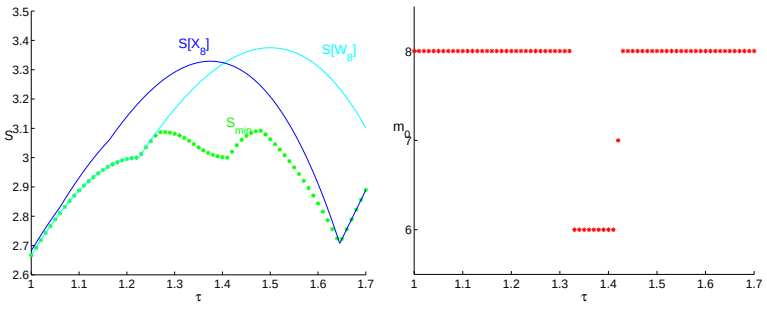



Figure 5.9: The minimal action for 8 points (left) and the number of distinct points(right).

**m = 12**: The solution of the Tammes problem is the icosahedron with minimal distance $\vartheta_{12} = \arccos\frac{1}{\sqrt{5}}$, concluding that

$$\tau_{12} = \frac{1}{2}(5 + \sqrt{5}) \approx 1.90211.$$

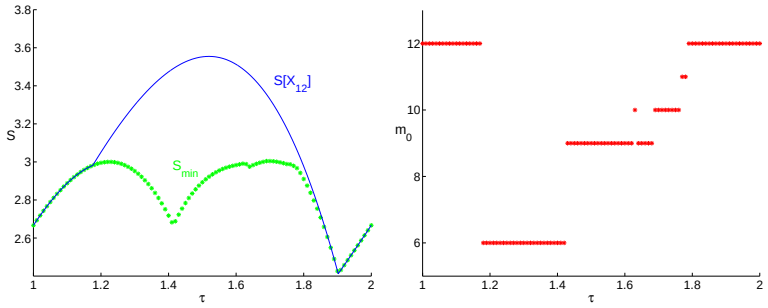



Figure 5.10: The minimal action for 12 points (left) and the number of distinct points(right).

Regarding the course of the minimal action varying $\tau$, see Figure 5.10, the minimal value of $\mathcal{S}_{\min}(\tau)$ for different values of $\tau$ is not attained at $\tau = 1$ but at $\tau = \tau_{12}$, thus $\mathcal{S}_{\min}(\tau = \tau_{12}) < \mathcal{S}_{\min}(\tau)$ for all $\tau \neq \tau_{12}$. Since $\sum_{x \in X_{12}} x = 0$, we conclude that the vectors of the icosahedron define a fermionic projector whose local correlation matrices have rank two. We compare this with the results of Section 4.4 in the case $m = 12$. Rescaling with the factor $\lambda = \frac{1}{12}$ yields that the action of the fermionic projector corresponding to the icosahedron configuration is given by

$$\mathcal{S}[P] = \frac{1}{12}\, 8\tau_{12}^2\, \lambda^4 \approx 0.0167502.$$

In accuracy of calculation, this fits together with the obtained minimal action of the variational principle on fermionic projectors. Now all distinct points are thus spacelike or lightlike separated, see Figure 5.11.

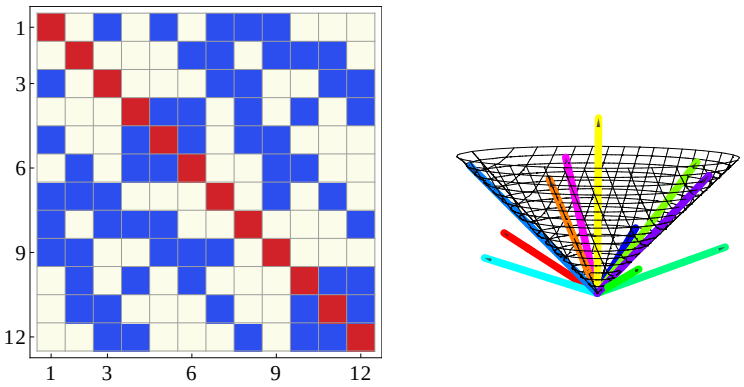


Figure 5.11: The plot of the matrix $\mathcal{D}$ and the Lorentzvectors on an exemplary base point $x$ corresponding to the icosahedron configuration.

We remark that in the cases $9 \leq m \leq 11$ similar effects like in the case $m = 8$ appeared, thus we skipped a detailed description. We remark that in the case $m = 11$ it is $\mathcal{S}_{\min}(\tau = 1) > \mathcal{S}_{\min}(\tau = \tau_{11})$, but the solution of the Tammes problem is the icosahedron less one point. Therefore this configuration does not require the constraint $\sum_{x \in X_{11}} x = 0$ and cannot be used to reconstruct a fermionic projector. If the

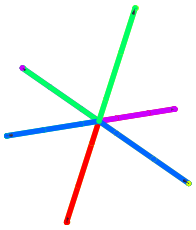


Figure 5.12: Clustering effect.

number of points is less than 11, it is always $\mathcal{S}_{\min}(\tau = 1) = \inf_\tau \mathcal{S}_{\min}(\tau)$. We conclude that in these cases, matrices of rank one yield the minimal action of the variational principle on matrices with prescribed varying eigenvalues given by (5.1.9). In this sense, the results of Section 4.4 appear to be reasonable.

## 5.5 The Transition to Causal Variational Principles on Measure Spaces

In the above numerical results, the number of distinct points $m_0$ was in some cases less than the given number $m$. The reason is that some of the points $x_i$ coincided, and form "clusters" of several points. Regarding exemplary the points in the case $m = 12$ and $\tau = 1.1$, see Figure 5.12, we observe only six distinct vectors, each of which appears twice in the minimal configuration. The multiple occupation of one single point $x_i$ can be interpreted as a weighting factor of the point $x_i$. If we compare the obtained results for different numbers of points, see Figure 5.13, one immediately sees that a higher number of points does not yield a lower action. Near $\tau \approx 1.2$, the plots for some values of $m$ look the same.

This "clustering effect" reveals that for large $m$ the minimizers might be well-approximated by a measure supported at few cluster points, with weights counting the number of points at each cluster. For any fixed $m \in \mathbb{N}$, we choose points $x_1, \ldots, x_m$ in $S^2$ and corresponding weights $\rho_1, \ldots, \rho_m$ with

$$\rho_i > 0 \qquad \text{and} \qquad \sum_{i=1}^m \rho_i = 1\,.$$

We introduce the *weighted counting measure* $\rho$ as

$$\rho = \sum_{i=1}^m \rho_i \delta_{x_i}, \tag{5.5.18}$$

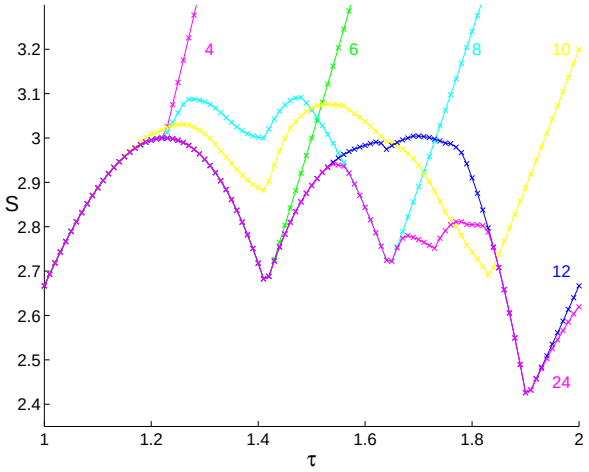



Figure 5.13: Numerical minima for the counting measure on the sphere.

where $\delta_x$ denotes the Dirac measure supported at the point $x \in S^2$. Thus $\rho$ satisfies the relation

$$\int_{S^2} f \, d\rho \;=\; \sum_{i=1}^{m} \rho_i \, f(x_i) \quad \text{for all} \quad f \in C^0(S^2)\,.$$

We define the set of finite weighted counting measures as

$$\mathfrak{M}_{count} = \left\{ \sum_{i=1}^{m} \rho_i \delta_{x_i} \;:\; m \in \mathbb{N},\; x_i \in S^2, \rho_i > 0,\; \sum_{i=1}^{m} \rho_i = 1 \right\},$$

which is a subset of the set of positive regular normalized (i.e. $\rho(S^2) = 1$) Borel measures on $S^2$, denoted by $\mathfrak{M}$. Defining the action of the measure $\rho \in \mathfrak{M}$ as

$$\mathcal{S}[\rho] = \iint_{S^2 \times S^2} \mathcal{L}(x,y) d\rho(x) d\rho(y), \tag{5.5.19}$$

the variational principle on measures is stated as

$$\boxed{\textbf{minimize } \mathcal{S}[\rho] \textbf{ by varying } \rho \in \mathfrak{M}.} \tag{5.5.20}$$

Regarding $\rho$ as a density on the sphere, the action (5.5.19) looks like the energy functional corresponding to a pair potential $\mathcal{L}$ (see for example [23]). Using physical notions, our pair potential is repelling (because $\mathcal{L}(\vartheta)$ is a decreasing function) and has short range (because $\mathcal{L}$ vanishes if $\vartheta \geq \vartheta_{\max}$). The action principle of Section 5.1 then corresponds to a variational principle on weighted counting measures with equal weighting factors $\rho_i = \frac{1}{m}$ for all $i = 1, \ldots, m$.

In the numerical approach, we regard the variational principle on measures (5.5.20) as a variational principle restricted on the subset $\mathfrak{M}_{count}$ of weighted counting measures supported at only a finite number of points. These satisfy the following approximation property:

**Lemma 5.5.** *The set of weighted counting measures $\mathfrak{M}_{count}$ is a dense subset of $\mathfrak{M}$ with regard to the weak $C^0(S^2)^*$-topology.*

*Proof.* Let $\nu \in \mathfrak{M}$. Since $S^2$ is compact, we can choose a partition of $S^2$ into $m$ subsets $K_1, \ldots, K_m$. For points $x_n \in K_n$, we set $\rho_m = \sum_{n=1}^m \nu(K_n) \delta_{x_n}$. We obtain

$$\lim_{m\to\infty} \int_{S^2} f(x)\, d\rho_m(x) = \int_{S^2} f(x)\, d\nu(x) \quad \text{for all} \quad f \in C^0(S^2),$$

which gives the claim. □

Since every normalized positive regular Borel measure $\rho$ can be approximated by counting measures $\rho_m$ given by (5.5.18), i.e. $\rho_m \to \rho$ for $m \to \infty$ with convergence in the weak $(C^0)^*$-topology, we can expect that if we choose $m$ sufficiently large, the obtained measure $\rho_m$ given by (5.5.18) should be a good approximation of a minimizing measure $\rho \in \mathfrak{M}$.

## 5.6 Solutions of Causal Variational Principles on Weighted Counting Measures

We next treat the variational principle on finite weighted counting measures numerically. In order to avoid constraints, we use spherical coordinates in $m$ dimensions: Each $\gamma \in S^{m-1}$ can uniquely be written as

$$\begin{aligned}
\gamma_1 &= \cos(\phi_1) \\
\gamma_2 &= \sin(\phi_1) \cos(\phi_2) \\
&\vdots \\
\gamma_{m-1} &= \sin(\phi_1) \sin(\phi_2) \ldots \cos(\phi_{m-1}) \\
\gamma_m &= \sin(\phi_1) \sin(\phi_2) \ldots \sin(\phi_{m-1})
\end{aligned}$$

for $\phi_i \in [0, \pi]$, $\phi_{m-1} \in [0, 2\pi)$. We again allow these scalars to obtain values in $\mathbb{R}$, only loosing the uniqueness of the representation. For $\gamma \in S^{m-1}$, we define the weighting factors $\rho_i$ of the counting measure given by (5.5.18) as

$$\rho_i = \gamma_i^2 \quad \text{for} \quad i \in \{1, \ldots, m\}.$$

The optimization problem differs by the dimension of the definition space and by the target function, but can in general be treated as described in section 5.3.

Now let $m \in \mathbb{N}$ be fixed. In the numerical study, we try to solve the variational principle (5.5.20) restricted on measures supported at most at $m$ points,

$$\text{minimize } \mathcal{S}[\rho] \text{ subject to } \rho = \sum_{i=1}^m \rho_i \delta_{x_i} \text{ with } \rho_i \geq 0, \sum_{i=1}^m \rho_i = 1,\ x_i \in S^2. \quad (5.6.21)$$

As starting point we use the measure $\rho_m$ supported at the spherical code $X_m$ that solves the Tammes problem with equal weighting factors, thus $\rho_m = \frac{1}{m} \sum_{x \in X_m} \delta_x$. In

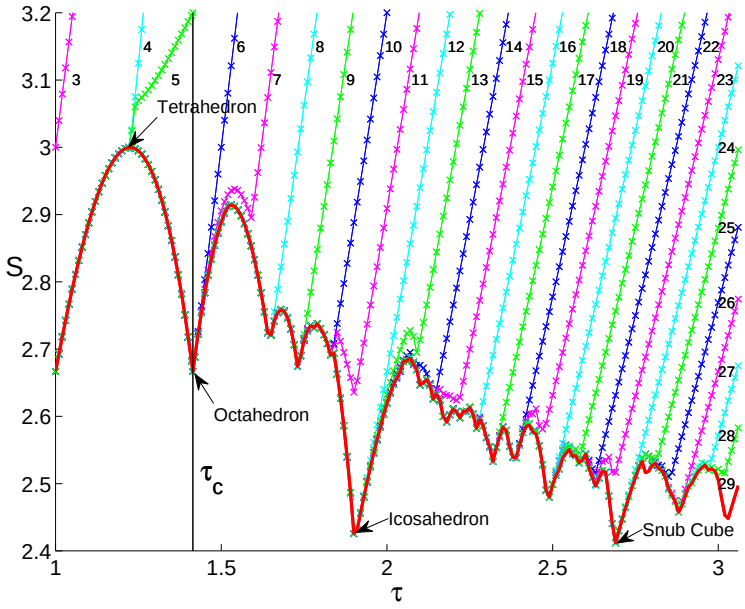



Figure 5.14: Numerical minima for the weighted counting measure on the sphere.

the case $\tau \geq \tau_m$, the measure $\rho_m$ solves the variational principle (5.6.21), as a simple calculation shows. The additional freedom in choosing the weighting factor does not always influence the minimal action: in the cases $m = 3, \ldots, 6$, the solutions of Section 5.4 with equal weighting factors are also the solutions of the weighted variational principle. Certainly, in general the action of the minimizing measure lies below the action with equal weighting factors.

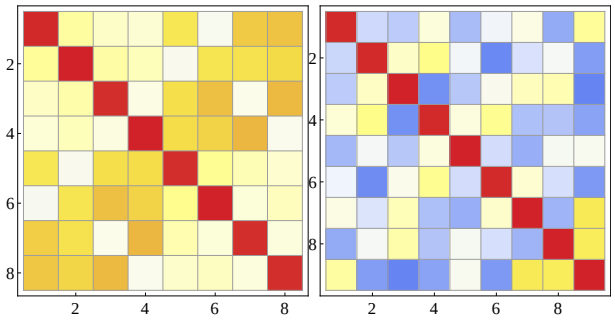
Combining the numerical minimal actions for different values of $m$, we obtain the plots shown in Figure 5.14. These plots suggest the following structure of the minimizers. Let us denote the minimizing weighted counting measure for a given $m$ by $\rho(m)$. Then for any fixed $\tau$, the series $\mathcal{S}[\rho(m)]$ is monotone decreasing (this is obvious because every $\rho(m)$ can be realized by a weighted counting measure with $m_+ > m$ summands by choosing $m_+ - m$ weights equal to zero). The important observation is that there is an integer $m_0$ from where on the series stays constant, i.e.

$$\mathcal{S}[\rho(m_-)] > \mathcal{S}[\rho(m_0)] = \mathcal{S}[\rho(m_+)] \qquad \forall\, m_- < m_0 < m_+ \,. \tag{5.6.22}$$

This implies that the measure $\rho_{m_0}$ is also a minimizer in the class of all Borel measures $\mathfrak{M}$. This leads us to the following

**Conjecture 5.6.** *For any $\tau \geq 1$, there is a minimizer $\rho \in \mathfrak{M}$ of the variational problem on the sphere which is a weighted counting measure supported at $m_0$ points.*

From Figure 5.14 we can read off the value of $m_0$ as a function of $\tau$. Generally speaking, $m_0$ increases as $\tau$ gets larger. This corresponds to the fact that for increasing $\tau$, the opening angle $\vartheta_{\max}$ of the light cones gets smaller, so that it becomes possible to distribute more points on the sphere which are all spatially separated from all the other points.




(a) $\tau = 1.2$ (b) $\tau = 1.7$

Figure 5.15: Plots of the matrix $\mathcal{D}$ for points in the support of $\rho(12)$ illustrating the phase transition.

The more detailed numerical study of the minimizers showed another interesting effect. For values $\tau < \tau_c := \sqrt{2}$, we found many different minimizers of different form. They all have the property that they are *completely timelike* in the sense that all points in the support of the minimizing measure have timelike or lightlike separation from all the other points, see Figure 5.15. We found minimizers supported on an arbitrarily large number of points. If on the other hand $\tau > \tau_c$, all minimizers were supported on at most $m_0(\tau)$ points, indicating that every minimizing measure $\rho \in \mathfrak{M}$ should be *discrete with finite support*. The intermediate value $\tau = \tau_c$ correspond to the opening angle $\vartheta_{\max} = \frac{\pi}{2}$ of the light cones.

**Conjecture 5.7.** *If $\tau < \tau_c$, every minimizer is completely timelike. If conversely $\tau > \tau_c$, every minimizing measure is discrete with finite support.*

More graphically, one can say that for $\tau > \tau_c$, our variational principle *spontaneously generates a discrete structure* on the sphere. The two regions $\tau < \tau_c$ and $\tau > \tau_c$ can also be understood as two different phases of the system, so that at $\tau = \tau_c$ we have a *phase transition* from the completely timelike phase to the discrete phase.

Taking a closer look on the minimizers in the case $\tau > \tau_c$, there occurs another interesting feature: If $\rho = \sum_{i=1}^{m} \rho_i \delta_{x_i}$ is the minimizing weighted counting measure, for each point $x_i$ there exists $x_j$ such that $\mathcal{D}(x_i, x_j) \approx 0$, see Figure 5.15. To be more precise, it is $\arccos(x_i \cdot x_j) = \vartheta_{\max}$, where $\vartheta_{\max}$ was defined in (5.1.11). Thus it seems that the point where the function $\mathcal{D}$ changes sign is of great importance.

Additionally, it seems that regular solids play an important role and distinguish from less regular solutions of the Tammes problem since AT these points, the course of the minimal action varying $\tau$ gets minimal, as indicated in Figure 5.14.

In Chapter 7, we will recur to the discussed variational principle on the sphere. Using the general structural results, we will try to prove the stated conjectures.

# 6 Structural Results on General Causal Variational Principles on Measure Spaces

## 6.1 The General Framework

We now introduce causal variational principles on measures in general framework, maintaining the important basic properties[1]. The numerical results of the variational principles on the sphere will be the guide line for the general analysis, where we refer to [8] for the used measure theoretic foundations and to [32] for the used functional analytic methods. The completely timelike phase will be analyzed in Section 6.4 using the notion of "generically timelike", whereas in Section 6.5 we will develop under which assumptions and in which sense the support of the minimizing measure is discrete or "singular". The phase transition is made precise in Theorems 6.19 and 6.21 by stating that minimizing measures are either generically timelike or singular.

Let $\mathcal{F}$ be a smooth compact manifold (of arbitrary dimension). We denote by $\mathfrak{M}$ the set of all normalized positive regular Borel measures on $\mathcal{F}$, where we call a measure $\rho$ normalized if $\rho(\mathcal{F}) = 1$. We introduce the support of a measure:

**Definition 6.1.** *The* ***support*** *of the measure $\rho \in \mathfrak{M}$ is defined as*

$$\text{supp}(\rho) = \{x \in \mathcal{F} \;:\; \rho(N) > 0 \;\; \textit{for every open neighborhood } N \textit{ of } x\}.$$

We remark that the support is a closed subset of $\mathcal{F}$.

The variational principles are stated as follows: For a function $\mathcal{D} \in C^\infty(\mathcal{F} \times \mathcal{F}, \mathbb{R})$

$$\text{being symmetric: } \mathcal{D}(x,y) = \mathcal{D}(y,x) \quad \text{for all } \; x, y \in \mathcal{F} \tag{6.1.1}$$
$$\text{and strictly positive on the diagonal: } \mathcal{D}(x,x) > 0\,, \tag{6.1.2}$$

we define the *Lagrangian* $\mathcal{L}$ by

$$\mathcal{L} = \max(0, \mathcal{D}) \in C^{0,1}(\mathcal{F} \times \mathcal{F}, \mathbb{R}^+_0)\,. \tag{6.1.3}$$

Introducing the *action* $\mathcal{S}$ by

$$\mathcal{S}[\rho] = \iint_{\mathcal{F}\times\mathcal{F}} \mathcal{L}(x,y)\, d\rho(x)\, d\rho(y)\,, \tag{6.1.4}$$

[1] This Chapter has already been published in [16]

our action principle is to

$$\boxed{\textbf{minimize } \mathcal{S}[\rho] \textbf{ under variations of } \rho \in \mathfrak{M}\,.} \tag{6.1.5}$$

In view of the symmetric form of (6.1.4), it is no loss of generality to assume that $\mathcal{L}(x,y)$ is symmetric in $x$ and $y$. Therefore, it is natural to assume that also $\mathcal{D}(x,y)$ is symmetric (6.1.1). If the condition (6.1.2) were violated, every measure supported in the set $\{x : \mathcal{D}(x,x) \leq 0\}$ would be a minimizer. Thus the condition (6.1.2) rules out trivial cases.

The existence of minimizers follows immediately from abstract compactness arguments (see [15, Section 1.2]).

**Theorem 6.2.** *The infimum of the variational principle* (6.1.5) *is attained in* $\mathfrak{M}$.

*Proof.* Let $C^0(\mathcal{F})$ be the Banach space of continuous real-valued functions on $\mathcal{F}$, equipped with the supremum norm $\|f\|_{C^0(\mathcal{F})} = \sup_{x\in\mathcal{F}} |f(x)|$. For $\nu$ in $\mathfrak{M}$, the corresponding linear positive continuous functional $I_\nu$, defined by

$$I_\nu : C^0(\mathcal{F}) \to \mathbb{R}, \quad I_\nu(f) = \int_{\mathcal{F}} f(x) d\nu(x),$$

satisfies due to the positivity and normalization of the measure $\nu$

$$\|I_\nu\|_{C^0(\mathcal{F})^*} = 1, \;\; I_\nu(1) = 1 \;\text{ and } I_\nu(f) \geq 0 \;\text{ for all }\; f \geq 0. \tag{6.1.6}$$

Let $(\rho_k)$ be a minimizing sequence of measures in $\mathfrak{M}$. According to the Theorem of Banach-Alaoglu, there exists a weak-$*$-convergent subsequence $(\mathcal{I}_{\rho_{n_k}})_k$ of $(I_{\rho_k})_k$. The limit defines a positive functional $I$ on $C^0(\mathcal{F})$, $I(f) := \lim_{k\to\infty} \rho_{n_k}(f)$. Using the Riesz representation theorem, there exists a positive regular measure $\rho$ on $\mathcal{F}$ such that

$$I(f) = \int_{\mathcal{F}} f(x) d\rho(x) \quad \text{for all} \quad f \in C^0(\mathcal{F}).$$

According to (6.1.6), it is $\rho(\mathcal{F}) = 1$, concluding that $\rho \in \mathfrak{M}$ . □

We note that the minimizers will in general not be unique. Moreover, the abstract framework gives no information on how the minimizers look like.

The notion of causality is again introduced via the sign of $\mathcal{D}$ with slightly difference in the definition of the boundary of the light-cone:

**Definition 6.3 (causal structure).**

$$\textit{Two points } x, y \in \mathcal{F} \textit{ are called } \left\{ \begin{array}{c} \textbf{\textit{timelike}} \\ \textbf{\textit{lightlike}} \\ \textbf{\textit{spacelike}} \end{array} \right\} \textit{ separated if } \left\{ \begin{array}{c} \mathcal{D}(x,y) > 0 \\ \mathcal{D}(x,y) = 0 \\ \mathcal{D}(x,y) < 0\,. \end{array} \right\}$$

*We define the sets*

$$\begin{aligned}
\mathcal{I}(x) &= \{y \in \mathcal{F} \text{ with } \mathcal{D}(x,y) > 0\} && \text{open light-cone} \\
\mathcal{J}(x) &= \{y \in \mathcal{F} \text{ with } \mathcal{D}(x,y) \geq 0\} && \text{closed light-cone} \\
\mathcal{K}(x) &= \partial\mathcal{I}(x) \cap \partial\big(\mathcal{F} \setminus \mathcal{J}(x)\big) && \text{boundary of the light-cone}\,.
\end{aligned}$$

Thus $y \in \mathcal{K}(x)$ if and only if the function $\mathcal{D}(x,.)$ changes sign in every neighborhood of $y$, the set $\mathcal{K}(x)$ differs from the set of lightlike separated points. The action is compatible with the causal structure in the sense that if $x$ and $y$ have lightlike or spacelike separation, then the Lagrangian vanishes, so that the pair $(x,y)$ does not contribute to the action. If $\rho$ is a given minimizer, we have similarly a causal structure on its support by restriction.

## 6.2 The Homogenizer of a Function

We begin the general studies with introducing some notation. For a given measure $\rho \in \mathfrak{M}$, we define the functions

$$\ell(x) = \int_{\mathcal{F}} \mathcal{L}(x,y)\, d\rho(y) \quad \in C^{0,1}(\mathcal{F}) \tag{6.2.7}$$

$$\mathsf{d}(x) = \int_{\mathcal{F}} \mathcal{D}(x,y)\, d\rho(y) \quad \in C^\infty(\mathcal{F})\,. \tag{6.2.8}$$

Moreover, we denote the Hilbert space $L^2(\mathcal{F}, d\rho)$ by $(\mathcal{H}_\rho, \langle .,. \rangle_\rho)$ and introduce the operators

$$\mathcal{L}_\rho \,:\, \mathcal{H}_\rho \to \mathcal{H}_\rho \,:\, \psi \mapsto (\mathcal{L}_\rho \psi)(x) = \int_{\mathcal{F}} \mathcal{L}(x,y)\, \psi(y)\, d\rho(y) \tag{6.2.9}$$

$$\mathcal{D}_\rho \,:\, \mathcal{H}_\rho \to \mathcal{H}_\rho \,:\, \psi \mapsto (\mathcal{D}_\rho \psi)(x) = \int_{\mathcal{F}} \mathcal{D}(x,y)\, \psi(y)\, d\rho(y)\,. \tag{6.2.10}$$

**Lemma 6.4.** *The operators $\mathcal{L}_\rho$ and $\mathcal{D}_\rho$ are self-adjoint and Hilbert-Schmidt. The eigenfunctions of $\mathcal{L}_\rho$ (and $D_\rho$) corresponding to the non-zero eigenvalues can be extended to Lipschitz-continuous (respectively smooth) functions on $\mathcal{F}$.*

*Proof.* We only consider $\mathcal{D}_\rho$, as the proof for $\mathcal{L}_\rho$ is analogous. The self-adjointness follows immediately from the fact that $\mathcal{D}(x,y)$ is symmetric. Moreover, as the kernel is smooth and $\mathcal{F}$ is compact, we know that

$$\iint_{\mathcal{F}\times\mathcal{F}} |\mathcal{D}(x,y)|^2 d\rho(x)\, d\rho(y) < \infty\,.$$

This implies that $\mathcal{D}_\rho$ is Hilbert-Schmidt (see [20, Theorem 2 in Section 16.1]). Suppose that $\mathcal{D}_\rho \psi = \lambda\psi$ with $\lambda \neq 0$. Then the representation

$$\psi(x) = \frac{1}{\lambda} \int_{\mathcal{F}} \mathcal{D}(x,y)\, \psi(y)\, d\rho(y)$$

shows that $\psi \in C^\infty(\mathcal{F})$. □

The following notions characterize properties of $\mathcal{F}$ and the function $\mathcal{D}$ which will be needed later on.

**Definition 6.5.** *A measure $\mu \in \mathfrak{M}$ is called* **homogenizer** *of the function $\mathcal{D}$ if* $\operatorname{supp}\mu = \mathcal{F}$ *and the functions*

$$\ell_\mu(x) := \int_{\mathcal{F}} \mathcal{L}(x,y)\, d\mu(y) \qquad \text{and} \qquad \mathsf{d}_\mu(x) := \int_{\mathcal{F}} \mathcal{D}(x,y)\, d\mu(y)$$

*are both constant on $\mathcal{F}$. The function $\mathcal{D}$ is called* **homogenizable** *if a homogenizer of $\mathcal{D}$ exists.*

In the application examples, $\mathcal{D}$ is a $G$-invariant function on the $G$-homogeneous space $\mathcal{F}$. Thus the homogenizer can in these cases be chosen as the normalized Haar measure on the homogeneous space $\mathcal{F}$, whose existence is discussed in [3, Section 1].

The next proposition gives a sufficient condition for a homogenizer to be a minimizer.

**Proposition 6.6.** *If $\mathcal{L}_\mu$ is a non-negative operator, the homogenizer $\mu$ is a minimizer of the variational principle* (6.1.5).

*Proof.* We denote the constant function on $\mathcal{F}$ by $1_{\mathcal{F}} \equiv 1$. If $\mu$ is a homogenizer, this function is an eigenfunction of $\mathcal{L}_\mu$, which can be completed to an orthonormal eigenvector basis $(\psi_i)_{i\in\mathbb{N}_0}$ of $\mathcal{H}_\mu$ with $\psi_0 = 1_{\mathcal{F}}$ and corresponding eigenvalues $\lambda_i \geq 0$. Using an approximation argument in the $C^0(\mathcal{F})^*$-topology, it suffices to show that

$$\mathcal{S}[\mu] \leq \mathcal{S}[\psi\mu]$$

for any $\psi \in C^0(\mathcal{F})$ with $\psi \geq 0$ and $\langle \psi, 1_{\mathcal{F}}\rangle_\mu = 1$. We write $\psi$ in the eigenvector basis $\psi_i$,

$$\psi = \sum_{i=0}^{\infty} c_i\, \psi_i\,.$$

The condition $\langle \psi, 1_{\mathcal{F}}\rangle_\mu = 1$ implies that $c_0 = 1$. Thus

$$\mathcal{S}[\psi\mu] = \langle \psi, \mathcal{L}_\mu \psi\rangle_\mu = \lambda_0 + \sum_{i=1}^{\infty} |c_i|^2 \lambda_i \geq \lambda_0 = \mathcal{S}[\mu]\,.$$

□

The converse of the above Proposition will be shown in the following section.

Studying the spectral properties of the operator $\mathcal{L}_\mu$, we can immediately state the homogenizer as minimizer. In most cases of course, the operator $\mathcal{L}_\mu$ fails to be non-negative.

## 6.3 The Euler-Lagrange Equations

Let $\rho \in \mathfrak{M}$ be a minimizer of the variational principle (6.1.5),

$$\mathcal{S}[\rho] = \inf_{\tilde{\rho} \in \mathfrak{M}} \mathcal{S}[\tilde{\rho}] =: \mathcal{S}_{\min} .$$

We now derive consequences of the minimality. In the first lemma, we consider first order variations of $\rho$ to obtain the Euler-Lagrange equations corresponding to our variational principle. The second lemma, on the other hand, accounts for a nonlinear effect.

**Lemma 6.7.** *(The Euler-Lagrange equations)*
*Let $\ell$ be the function* (6.2.7) *relating to the minimizing measure $\rho$. Then $\ell$ satisfies the equations*

$$\ell|_{\text{supp}\,\rho} \equiv \inf_{\mathcal{F}} \ell = \mathcal{S}_{\min} .$$

*Proof.* Comparing (6.1.4) with (6.2.7), one sees that

$$\mathcal{S}_{\min} = \int_{\mathcal{F}} \ell \, d\rho . \tag{6.3.11}$$

Since $\ell$ is continuous and $\mathcal{F}$ is compact, there clearly is $y \in \mathcal{F}$ with

$$\ell(y) = \inf_{\mathcal{F}} \ell . \tag{6.3.12}$$

We consider for $t \in [0,1]$ the family of measures

$$\tilde{\rho}_t = (1-t)\,\rho + t\,\delta_y \;\in \mathfrak{M} ,$$

where $\delta_y$ denotes the Dirac measure at $y$. Substituting this formula in (6.1.4) and differentiating, we obtain for the first variation the formula

$$\delta\mathcal{S} := \lim_{t \searrow 0} \frac{\mathcal{S}[\tilde{\rho}_t] - \mathcal{S}[\tilde{\rho}_0]}{t} = -2\mathcal{S}_{\min} + 2\ell(y) .$$

Since $\rho$ is a minimizer, $\delta\mathcal{S}$ is non-negative. Combining this result with (6.3.11) and (6.3.12), we obtain the relations

$$\inf_{\mathcal{F}} \ell = \ell(y) \;\geq\; \mathcal{S}_{\min} = \int_{\mathcal{F}} \ell \, d\rho .$$

It follows that $\ell$ is constant on the support of $\rho$, giving the result. □

**Lemma 6.8.** *The operator $\mathcal{L}_\rho$ is non-negative.*

*Proof.* Lemma (6.7) yields that for any $x \in \operatorname{supp}\rho$,

$$(\mathcal{L}_\rho 1_\mathcal{F})(x) = \int_\mathcal{F} \mathcal{L}(x,y)\, d\rho(y) = \ell(x) = \mathcal{S}_{\min}\, 1_\mathcal{F}(x)\,,$$

showing that the constant function $1_\mathcal{F}$ is an eigenvector corresponding to the eigenvalue $\mathcal{S}_{\min} \geq 0$.

Assume that the lemma is wrong. Then, as $\mathcal{L}_\rho$ is a compact and self-adjoint operator (see Lemma 6.4), there exists an eigenvector $\psi$ corresponding to a negative eigenvalue, $\mathcal{L}_\rho \psi = \lambda\psi$ with $\lambda < 0$. We consider the family of measures

$$\tilde\rho_t = (1_\mathcal{F} + t\psi)\,\rho\,.$$

In view of Lemma 6.4, $\psi$ is continuous and therefore bounded. Thus for sufficiently small $|t|$, the measure $\tilde\rho_t$ is positive. Moreover, the orthogonality of the eigenfunctions $1_\mathcal{F}$ and $\psi$ implies that

$$\tilde\rho_t(\mathcal{F}) = \int_F 1_\mathcal{F}\,(1_\mathcal{F} + t\psi)\, d\rho = 1 + t\,\langle 1_\mathcal{F}, \psi\rangle_\rho = 1\,,$$

showing that $\tilde\rho_t$ is again normalized. Finally, again using the orthogonality,

$$\mathcal{S}[\tilde\rho_t] = \langle (1_\mathcal{F} + t\psi), L_\rho(1_\mathcal{F} + t\psi)\rangle_\rho = \mathcal{S}_{\min} + \lambda\, t^2\, \langle\psi,\psi\rangle_\rho\,.$$

Thus $\tilde\rho_t$ is an admissible variation which decreases the action, a contradiction. □

An immediate consequence of this lemma is a useful positivity property of the Lagrangian when evaluated on a finite number of points in the support of $\rho$.

**Corollary 6.9.** *For a finite family $x_0, \ldots, x_N \in \operatorname{supp}\rho$ (with $N \in \mathbb{N}$), the **Gram matrix** $L$ defined by*

$$L = \Big(\mathcal{L}(x_i, x_j)\Big)_{i,j=0,\ldots,N}$$

*is symmetric and positive semi-definite.*

*Proof.* Given $\varepsilon > 0$ and a vector $u = (u_0, \ldots, u_N) \in \mathbb{C}^{N+1}$, we set

$$\psi_\epsilon(x) = \sum_{i=0}^N \frac{u_i}{\rho(B_\varepsilon(x_i))}\, \chi_{B_\varepsilon(x_i)}(x) \in \mathcal{H}_\rho\,,$$

where $B_\varepsilon$ is a ball of radius $\varepsilon$ (in a given coordinate system). Lemma 6.8 implies that $\langle \psi_\varepsilon, \mathcal{L}_\rho \psi_\varepsilon\rangle \geq 0$. Taking the limit $\varepsilon \searrow 0$, it follows that

$$\langle u, Lu\rangle_{\mathbb{C}^{N+1}} = \lim_{\varepsilon\searrow 0} \langle \psi_\varepsilon, \mathcal{L}_\rho\psi_\varepsilon\rangle_\rho \geq 0\,.$$

□

Finally, the Euler-Lagrange equations yield a first property of the support of the minimizing measure.

**Lemma 6.10.** *If the homogenizer $\mu$ does not solve* (6.1.5)*, then $\mu(\mathcal{F}\setminus \operatorname{supp}\rho) > 0$.*

*Proof.* The function $\ell_\mu$ is constant with $\ell_\mu(x) \equiv \ell_\mu > \mathcal{S}_{\min}$. Using Lemma 6.7, one can estimate

$$\ell_\mu = \iint_{\mathcal{F}\times\mathcal{F}} \mathcal{L}(x,y) d\mu(x) d\rho(y) = \int_\mathcal{F} \ell_\rho(x) d\mu(x) > \mathcal{S}_{\min} = \int_\mathcal{F} \ell_\rho(x) d\rho(x),$$

concluding there exists $U \subset \mathcal{F}$ with $\mu(U) > 0$ but $\rho(U) = 0$. □

## 6.4 Generically Timelike Minimizers

Motivated by the observed phase transition, we now introduce an outstanding class of minimizing measures and discuss its existence:

**Definition 6.11.** *A minimizing measure $\rho \in \mathfrak{M}$ is called* **generically timelike** *if the following conditions hold:*

*(i)* $\mathcal{D}(x,y) \geq 0$ *for all* $x, y \in \operatorname{supp} \rho$.

*(ii) The function* $\mathsf{d}$ *defined by* (6.2.8) *is constant on* $\mathcal{F}$.

This constant can easily be computed.

**Lemma 6.12.** *Suppose that $\rho$ is a generically timelike minimizer. Then*

$$\mathsf{d}(x) = \mathcal{S}_{\min} \qquad \text{for all } x \in \mathcal{F}\,.$$

*Proof.* Since the measure $\rho$ is generically timelike, the function $\mathcal{D}$ is positive on the support of $\rho$. Consequently, the functions $\mathcal{L}$ and $\mathcal{D}$ coincide on the support of $\rho$, yielding

$$\mathcal{S}_{\min} = \iint_{\mathcal{F}\times\mathcal{F}} \mathcal{L}(x,y)\, d\rho(x)\, d\rho(y) = \iint_{\mathcal{F}\times\mathcal{F}} \mathcal{D}(x,y)\, d\rho(x)\, d\rho(y)\,.$$

Carrying out one integral using (6.2.8), we obtain

$$\mathcal{S}_{\min} = \int_{\mathcal{F}} \mathsf{d}(x)\, d\rho(x)\,,$$

giving the result. □

In the remainder of this subsection, we assume that $\mathcal{D}$ is homogenizable (see Definition 6.5) and denote the homogenizer by $\mu \in \mathfrak{M}$.

**Lemma 6.13.** *If $\mathcal{D}_\mu$ has only a finite number of negative eigenvalues, the kernel $\mathcal{D}(x,y)$ has the representation*

$$\mathcal{D}(x,y) = \nu_0 + \sum_{n=1}^{N} \nu_n\, \phi_n(x)\, \overline{\phi_n(y)} \tag{6.4.13}$$

*with $N \in \mathbb{N} \cup \{\infty\}$, $\nu_n \in \mathbb{R}$, $\nu_n \neq 0$, and $\phi_n \in C^\infty(\mathcal{F})$, where in the case $N = \infty$ the series converges uniformly.*

*Proof.* By definition of the homogenizer, the function $1_{\mathcal{F}} \equiv 1$ is an eigenfunction of the operator $\mathcal{D}_\mu$. Denoting the corresponding eigenvalue by $\nu_0$, we obtain the spectral representation (6.4.13).

If $\mathcal{D}_\mu$ is positive semi-definite, the uniform convergence is an immediate generalization of Mercer's theorem (see [20, Theorem 11 in Chapter 30], where we replace

the interval $[0,1]$ by the compact space $\mathcal{F}$, and the Lebesgue measure by the measure $\mu$). In the case when $\mathcal{D}_\mu$ has a finite number of negative eigenvalues, we apply Mercer's theorem similarly to the operator with kernel $\mathcal{D}(x,y) - \sum_{i=1}^K \lambda_i\, \psi_i(x) \overline{\psi_i(y)}$, where $\lambda_1, \ldots \lambda_K$ are the negative eigenvalues with corresponding eigenfunctions $\psi_i$. By construction, this operator is positive semi-definite, and in view of Lemma 6.4 its kernel is continuous. □

**Lemma 6.14.** *Suppose that $\rho$ is a generically timelike minimizer and that the operator $\mathcal{D}_\mu$ has only a finite number of negative eigenvalues. Then*

$$\mathcal{S}[\rho] = \nu_0 \qquad \text{and} \qquad \int_{\mathcal{F}} \phi_n(y)\, d\rho(y) = 0 \quad \text{for all } n \in \{1, \ldots, N\}\,.$$

*Proof.* Using the decomposition of the kernel (6.4.13) and the uniform convergence, we obtain

$$\mathsf{d}(x) = \nu_0 + \sum_{n=1}^N \nu_n\, \phi_n(x) \int_{\mathcal{F}} \overline{\phi_n(y)}\, d\rho(y)\,.$$

Applying Lemma 6.12 gives the claim. □

**Proposition 6.15.** *Suppose that $\mathcal{D}_\mu$ is a positive semi-definite operator on $\mathcal{H}_\mu$. Let $\nu_0$ denote the eigenvalue corresponding to the constant function $1_{\mathcal{F}}$. Then*

$$\mathcal{S}_{\min} \geq \nu_0\,.$$

*In the case of equality, every minimizer is generically timelike.*

*Proof.* If $\mathcal{D}_\mu$ is positive semi-definite, all the parameters $\nu_n$ in (6.4.13) are positive. It follows that for every measure $\tilde\rho \in \mathfrak{M}$,

$$\mathcal{S}[\tilde\rho] = \iint_{\mathcal{F}\times\mathcal{F}} \mathcal{L}(x,y)\, d\tilde\rho(x)\, d\tilde\rho(y) \geq \iint_{\mathcal{F}\times\mathcal{F}} \mathcal{D}(x,y)\, d\tilde\rho(x)\, d\tilde\rho(y) \geq \nu_0\, \tilde\rho(\mathcal{F})^2 = \nu_0\,. \tag{6.4.14}$$

Let us assume that equality holds. It then follows from (6.4.14) that $\mathcal{L}$ and $\mathcal{D}$ coincide on the support of $\tilde\rho$ and thus $\mathcal{D}(x,y) \geq 0$ for all $x, y \in \operatorname{supp}\tilde\rho$. Moreover, we find from (6.4.13) that

$$\nu_0 = \nu_0 + \sum_{n=1}^N \left| \int_{\mathcal{F}} \overline{\phi_n(y)}\, d\tilde\rho \right|^2,$$

and thus

$$\int_{\mathcal{F}} \overline{\phi_n(y)}\, d\tilde\rho = 0 \qquad \text{for all } n \geq 1\,.$$

It follows that $\mathsf{d}_{\tilde\rho}$ is a constant. We conclude that $\tilde\rho$ is generically timelike. □

This proposition can be used to construct generically timelike minimizers:

**Corollary 6.16.** *Suppose that $\mathcal{D}_\mu$ is a positive semi-definite operator on $\mathcal{H}_\mu$. Assume that the function $f \in \mathcal{H}_\mu$ has the following properties:*

*(a)* $\mathcal{D}(x,y) = \mathcal{L}(x,y)$ *for all* $x, y \in \operatorname{supp} f$.

*(b)* $\displaystyle\int_{\mathcal{F}} f(x)\, d\mu(x) = 1 \quad \text{and} \quad \int_{\mathcal{F}} f(x)\, \phi_n(x)\, d\mu(x) = 0 \quad \text{for all } n \in \{1, \ldots, N\}.$

*Then the measure $d\rho = f\, d\mu$ is a generically timelike minimizer.*

*Proof.* The assumption (a) implies that

$$\mathcal{S}[\rho] = \iint_{\mathcal{F}\times\mathcal{F}} \mathcal{D}(x,y)\, d\rho(x)\, d\rho(y)\,.$$

Using the decomposition (6.4.13) and the relations (b), we find that $\mathcal{S}[\rho] = \nu_0$. We now apply Proposition 6.15. □

Consequently, if the operator $\mathcal{D}_\mu$ is positive semi-definite of finite rank, there exists a wide and rich family of generically timelike minimizers.

We conclude this section by stating obstructions for the existence of generically timelike minimizers.

**Proposition 6.17.** *Assume that one of the following conditions hold:*

*(I) The operator $\mathcal{D}_\mu$ has only a finite number of negative eigenvalues, and the eigenvalue $\nu_0$ in the decomposition* (6.4.13) *is not positive.*

*(II) For every $x \in \mathcal{F}$ there is a point $y \in \mathcal{F}$ with $\mathcal{J}(x) \cap \mathcal{J}(y) = \varnothing$ ("condition of disjoint light-cones").*

*(III) For every $x \in \mathcal{F}$ there is a point $-x \notin \overline{\mathcal{I}(x)}$ with $\mathcal{J}(x) = \overline{\mathcal{I}(x)} \cup \{-x\}$ and $\overline{\mathcal{I}(x)} \cap \overline{\mathcal{I}(-x)} = \varnothing$ ("condition of antipodal points").*

*Then there are no generically timelike minimizers.*

*Proof.* We first show that $\mathcal{S}_{\min} > 0$. Namely, choosing $x$ in the support of a minimizing measure $\rho$, we know from (6.1.2) and the continuity of $\mathcal{D}$ that there is a neighborhood $U$ of $x$ and $\delta > 0$ such that $\mathcal{D}(x,y) > \delta$ for all $y \in U$. It follows that

$$\mathcal{S}_{\min} \geq \int_{U\times U} \mathcal{L}(x,y)\, d\rho(x)\, d\rho(y) \geq \delta\, \rho(U)^2 > 0\,.$$

Case (I) is obvious in view of Lemma 6.14 and the fact that $\mathcal{S}_{\min} > 0$. To prove the remaining cases (II) and (III), we assume conversely that there exists a generically timelike minimizer $\rho \in \mathfrak{M}$. Choosing a point $x \in \operatorname{supp}\rho$, we know from property (i) in Definition 6.11 that $\operatorname{supp}\rho \subset \mathcal{J}(x)$. In case (II), we choose $y \in \mathcal{F}$ with $\mathcal{J}(x) \cap \mathcal{J}(y) = \varnothing$ to obtain

$$\mathsf{d}(y) = \int_{\mathcal{J}(x)} \mathcal{D}(y,z)\, d\rho(z) \leq 0 < \mathcal{S}_{\min}\,,$$

in contradiction to Lemma 6.12.

In case (III), we know that $\operatorname{supp}\rho \subset \mathcal{J}(x) = \overline{\mathcal{I}(x)} \cup \{-x\}$. If $-x \notin \operatorname{supp}\rho$, the estimate

$$\mathsf{d}(-x) = \int_{\mathcal{J}(x)} \mathcal{D}(-x,z)\,d\rho(z) = \int_{\overline{\mathcal{I}(x)}} \mathcal{D}(-x,z)\,d\rho(z) \overset{(*)}{\leq} 0 < \mathcal{S}_{\min}$$

again gives a contradiction, where in (*) we used that $\overline{\mathcal{I}(x)} \cap \overline{\mathcal{I}(-x)} = \varnothing$. If conversely $-x \in \operatorname{supp}\rho$, then $\operatorname{supp}\rho \subset \mathcal{J}(x) \cap \mathcal{J}(-x) = \{x\} \cup \{-x\}$ (where we again used that $\overline{\mathcal{I}(x)} \cap \overline{\mathcal{I}(-x)} = \varnothing$). Hence the integral in (6.2.8) reduces to a sum over two points,

$$\mathsf{d}(y) = \rho(\{x\})\,\mathcal{D}(y,x) + \rho(\{-x\})\,\mathcal{D}(y,-x)\,. \tag{6.4.15}$$

In view of our assumption (6.1.2), we know that $x \in \mathcal{I}(x)$. On the other hand, the relation $\overline{\mathcal{I}(x)} \cap \overline{\mathcal{I}(-x)} = \varnothing$ shows that $-x \notin \mathcal{I}(x)$. Hence there is a point $y \in \partial\mathcal{I}(x)$. It follows that $\mathcal{D}(y,x) = 0$ (because $y \in \partial\mathcal{I}(x)$) and also $\mathcal{D}(y,-x) \leq 0$ (because $y \in \overline{\mathcal{I}(x)}$ and thus $y \notin \overline{\mathcal{I}(-x)}$). Using these inequalities in (6.4.15), we again find that $\mathsf{d}(y) \leq 0$, a contradiction. □

It is an interesting question how the support of a generically timelike minimizer $\rho$ may look like. The next proposition (which will not be used later on) quantifies that $\operatorname{supp}\rho$ must be sufficiently "spread out".

**Proposition 6.18.** *Assume that $\rho$ is a generically timelike minimizer and that the operator $\mathcal{D}_\mu$ has only a finite number of negative eigenvalues. Then every real function $\psi \in \mathcal{D}_\mu(\mathcal{H}_\mu)$ with*

$$\int_{\mathcal{F}} \psi(x)\,d\mu(x) = 0 \tag{6.4.16}$$

*changes its sign on the support of $\rho$ (here $\mu$ is again the homogenizer of Definition 6.5).*

*Proof.* We return to the spectral decomposition (6.4.13) of the operator $\mathcal{D}_\mu$. Since the eigenfunctions $\phi_n$ are orthogonal in $\mathcal{H}_\mu$, we know that

$$\int_{\mathcal{F}} \phi_n\,d\mu = 0 \qquad \text{for all } n \geq 1\,.$$

Representing $\psi$ in an eigenvector basis of $\mathcal{D}_\mu$ and using (6.4.16), we find

$$\psi = \sum_{n=1}^{N} \kappa_n\,\phi_n$$

with complex coefficients $\kappa_n$. Integrating with respect to $\rho$, we can apply Lemma 6.14 to obtain

$$\int_{\mathcal{F}} \psi(x)\,d\rho(x) = \sum_{n=1}^{N} \kappa_n \int_{\mathcal{F}} \phi_n(x)\,d\rho(x) = 0\,.$$

Hence $\psi$ changes its sign on the support of $\rho$. □

## 6.5 Minimizers with Singular Support

We now state results on the support of a minimizing measure.

**Theorem 6.19.** *Let $\mathcal{F}$ be a smooth compact manifold. Assume that $\mathcal{D}(x,y)$ is symmetric* (6.1.1) *and equal to one on the diagonal, $\mathcal{D}(x,x) \equiv 1$. Furthermore, we assume that for every $x \in \mathcal{F}$ and $y \in \mathcal{K}(x)$, there is a smooth curve $c$ joining the points $x$ and $y$, along which $\mathcal{D}(.,y)$ has a non-zero derivative at $x$, i.e.*

$$\frac{d}{dt} \mathcal{D}\big(c(t), y\big)\Big|_{t=0} \neq 0\,, \tag{6.5.17}$$

*where we parametrized the curve such that $c(0) = x$. Then the following statements are true:*

*(A) If $\mathcal{F}$, $\mathcal{D}$ are real analytic, then a minimizing measure $\rho$ is either generically timelike or $\overset{\circ}{\text{supp}}\, \rho = \varnothing$.*

*(B) If $\mathcal{D}$ is smooth and if there is a differential operator $\Delta$ on $C^\infty(\mathcal{F})$ which vanishes on the constant functions such that*

$$\Delta_x \mathcal{D}(x,y) < 0 \qquad \text{for all } y \in \mathcal{I}(x)\,, \tag{6.5.18}$$

*then $\overset{\circ}{\text{supp}}\, \rho = \varnothing$.*

A typical example for $\Delta$ is the Laplacian corresponding to a Riemannian metric on $\mathcal{F}$. Note that the condition (6.5.17) implies that for every $y \in \mathcal{F}$, the set $\{x : y \in \mathcal{K}(x)\}$ is a smooth hypersurface, which the curve $c$ intersects transversely (in the applications of Chapter 7, this set will coincide with $\mathcal{K}(y)$, but this does not need to be true in general).

The condition (6.5.17) can be removed if instead we make the following symmetry assumption.

**Definition 6.20.** *The function $\mathcal{D}$ is called* ***locally translation symmetric*** *at $x$ with respect to a curve $c(t)$ with $c(0) = x$ if there is $\varepsilon > 0$ and a function $f \in C^\infty((-2\varepsilon, 2\varepsilon))$ such that the curve $c$ is defined on the interval $(-\varepsilon, \varepsilon)$ and*

$$\mathcal{D}(c(t), c(t')) = f(t - t') \qquad \text{for all } t, t' \in (-\varepsilon, \varepsilon)\,.$$

**Theorem 6.21.** *Let $\mathcal{F}$ be a smooth compact manifold. Assume that $\mathcal{D}(x,y)$ is symmetric* (6.1.1) *and strictly positive on the diagonal* (6.1.2)*. Furthermore, we assume that for every $x \in \mathcal{F}$ and $y \in \mathcal{K}(x)$, there is a smooth curve $c$ joining the points $x$ and $y$ such that $\mathcal{D}$ is locally translation symmetric at $x$ with respect to $c$, and such that the function $\mathcal{D}(c(t), y)$ changes sign at $t = 0$ (where we again parametrize the curve such that $c(0) = x$). Then statement (A) of Theorem 6.19 holds, provided that the curve $c$ is analytic in a neighborhood of $t = 0$. Assume furthermore that there is $p \in \mathbb{N}$ with*

$$\frac{d^p}{dt^p} \mathcal{D}\big(c(t), y\big)\Big|_{t=0} \neq 0\,. \tag{6.5.19}$$

*Then statement (B) of Theorem 6.19 again holds.*

In the smooth setting, the above theorems involve quite strong additional assumptions (see (6.5.17), (6.5.18) and (6.5.19)). The following counter example shows that some conditions of this type are necessary for the statements of these theorems to be true[2].

*Example* 6.22. *Let $f, g \in C_0^\infty([-\pi, \pi])$ be non-negative even functions with*

$$\operatorname{supp} f \subset \left[-\tfrac{\pi}{8}, \tfrac{\pi}{8}\right] , \qquad \operatorname{supp} g \subset \left(-\pi, -\tfrac{\pi}{2}\right] \cup \left[\tfrac{\pi}{2}, \pi\right) .$$

*We introduce the function $\mathcal{D} \in C^\infty(S^2 \times S^2)$ by*

$$\mathcal{D}(x,y) = -g\big(\operatorname{dist}(x,y)\big) + \int_{S^2} f\big(\operatorname{dist}(x,z)\big)\, f\big(\operatorname{dist}(z,y)\big)\, d\mu(z) , \tag{6.5.20}$$

*where $d\mu$ is the standard volume measure, and* dist *denotes the geodesic distance (taking values in $[0, \pi]$). Note that the two summands in* (6.5.20) *have disjoint supports and thus the corresponding Lagrangian* (6.1.3) *simply is*

$$\mathcal{L}(x,y) = \int_{S^2} f\big(\operatorname{dist}(x,z)\big)\, f\big(\operatorname{dist}(z,y)\big)\, d\mu(z) , \tag{6.5.21}$$

*We again consider $\mathcal{D}(x,y)$ and $\mathcal{L}(x,y)$ as the integral kernels of corresponding operators $\mathcal{D}_\mu$ and $\mathcal{L}_\mu$ on the Hilbert space $\mathcal{H}_\mu = L^2(S^2, d\mu)$.*

*First, it is obvious that $\mathcal{D}(x,y)$ is symmetric and constant on the diagonal. Next, it is clear by symmetry that the measure $\mu$ is a homogenizer (see Definition 6.5). Moreover, writing $\mathcal{L}_\mu$ as $\mathcal{L}_\mu = f_\mu^2$, where $f_\mu$ is the operator with integral kernel $f$, one sees that the operator $\mathcal{L}_\mu$ is non-negative. Thus by Proposition 6.6, the measure $\mu$ is minimizing. If the function $g$ is non-trivial, there are points $x, y$ which are spacelike separated, so that this minimizer is not generically timelike. Also, its support obviously has a non-vanishing interior. We have thus found a minimizing measure which violates statement (A) of Theorem 6.19.* ◊

The remainder of this section is devoted to the proof of the above theorems. We begin with a simple but very useful consideration. Suppose that for given $x \in \mathcal{F}$, the boundary of the light cone $\mathcal{K}(x)$ does not intersect the support of $\rho$. As the support of $\rho$ is compact, there is neighborhood $U$ of $x$ such that

$$\mathcal{K}(z) \cap \operatorname{supp} \rho = \varnothing \qquad \text{for all } z \in U .$$

Thus introducing the measure $\hat{\rho} = \chi_{\mathcal{I}(x)}\, \rho$, the function $\ell$ can for all $z \in U$ be represented by

$$\ell(z) = \int_{\mathcal{F}} \mathcal{L}(z,\xi)\, d\hat{\rho}(\xi) = \int_{\mathcal{F}} \mathcal{D}(z,\xi)\, d\hat{\rho}(\xi) . \tag{6.5.22}$$

This identity can be used both in the smooth and in the analytic case.

**Lemma 6.23.** *If* (6.5.18) *holds, then for every $x \in \operatorname{supp} \rho$ the set $\mathcal{K}(x) \cap \operatorname{supp} \rho$ is nonempty.*

[2] We would like to thank Robert Seiringer for pointing out a similar example to us.

*Proof.* Applying the differential operator $\Delta$ to (6.5.22) gives

$$\Delta_x \ell(x) = \int_{\mathcal{F}} \Delta_x \mathcal{D}(x,z)\, d\hat{\rho}(z) < 0\,,$$

where in the last step we used (6.5.18) and the fact that $x \in \operatorname{supp}\rho$. This is a contradiction to Lemma 6.7. □

**Lemma 6.24.** *Suppose that $\mathcal{F}$ and $\mathcal{D}$ are real analytic. Assume that there exists a point $x \in \overset{\circ}{\operatorname{supp}}\,\rho$ such that $\mathcal{K}(x) \cap \operatorname{supp}\rho = \varnothing$. Then $\rho$ is generically timelike and $\operatorname{supp}\rho \subset \mathcal{I}(x)$.*

*Proof.* We introduce on $\mathcal{F}$ the function

$$\hat{\mathsf{d}}(y) = \int_{\mathcal{F}} \mathcal{D}(y,z)\, d\hat{\rho}(y)\,.$$

Then $\hat{\mathsf{d}}$ is real analytic and, according to (6.5.22), it coincides on $U$ with the function $\ell$. Since $x \in \overset{\circ}{\operatorname{supp}}\,\rho$, the Euler-Lagrange equations in Lemma (6.7) yield that $\ell \equiv \mathcal{S}_{\min}$ in a neighborhood of $x$. Hence $\hat{\mathsf{d}} \equiv \mathcal{S}_{\min}$ in a neighborhood of $x$, and the real analyticity implies that

$$\hat{\mathsf{d}} \equiv \mathcal{S}_{\min} \qquad \text{on } \mathcal{F}\,.$$

It follows that

$$\begin{aligned} \mathcal{S}_{\min} &= \int_{\mathcal{F}} \hat{\mathsf{d}}(x) d\rho(x) = \iint_{\mathcal{F}\times\mathcal{F}} \mathcal{D}(x,y)\, d\hat{\rho}(x)\, d\rho(y) \\ &\leq \iint_{\mathcal{F}\times\mathcal{F}} \mathcal{L}(x,y)\, d\hat{\rho}(x)\, d\rho(y) = \int_{\mathcal{F}} \ell(x)\, d\hat{\rho}(x) = \mathcal{S}_{\min}\, \hat{\rho}(\mathcal{F})\,, \end{aligned} \tag{6.5.23}$$

and thus $\hat{\rho}(\mathcal{F}) = 1$. Since $\hat{\rho} \leq \rho$ and $\rho$ is normalized, we conclude that $\rho = \hat{\rho}$. Thus $\mathsf{d} \equiv \hat{\mathsf{d}} \equiv \mathcal{S}_{\min}$. Moreover, the inequality in (6.5.23) becomes an equality, showing that $\mathcal{L} \equiv \mathcal{D}$ on the support of $\rho$. Thus $\rho$ is indeed generically timelike. □

**Corollary 6.25.** *Assume that the conditions of Lemma 6.24 hold. If for $x \in \mathcal{F}$ there exists $y \in \mathcal{F}$ such that $\mathcal{I}(x) \cap \mathcal{I}(y) = \varnothing$, then $\overset{\circ}{\operatorname{supp}}\,\rho = \varnothing$.*

*Proof.* According to Lemma 6.24, the measure $\rho$ is generically timelike with $\operatorname{supp}\rho \subset \mathcal{I}(x)$. But for $y \in \mathcal{F}$ with $\mathcal{I}(x) \cap \mathcal{I}(y) = \varnothing$, one obtains

$$\ell(y) = \int_{\mathcal{I}(x)} \mathcal{L}(y,z) d\rho(z) = 0 < \mathcal{S}_{\min}$$

in contradiction to Lemma 6.7. □

To complete the proof of Theorems 6.19 and 6.21, it remains to show the following statement:

$$\mathcal{K}(x) \cap \operatorname{supp} \rho = \varnothing \qquad \text{for all } x \in \overset{\circ}{\operatorname{supp}}\, \rho\,. \tag{6.5.24}$$

We proceed indirectly and assume that there is a point $y \in \mathcal{K}(x) \cap \operatorname{supp} \rho$. Our strategy is to choose points $x_0, \ldots, x_k$ in a neighborhood of $x$ such that $\mathcal{L}$ restricted to the set $\{x_0, \ldots, x_k, y\}$ is not positive semi-definite, in contradiction to Corollary 6.9. The points $x_0, \ldots, x_k$ will all lie on a fixed smooth curve $c$ which joins $x$ and $y$ and is chosen as in the statement of the theorems. We parametrize $c$ such that $c(0) = x$ and $c(1) = y$, and by extending the curve we can arrange (possibly by decreasing $\varepsilon$) that the curve is defined on the interval $(-k\varepsilon, 1]$. By the assumptions in Theorems 6.19 and 6.21, we know that $\mathcal{D}(c(t), y)$ changes sign at $t = 0$. Depending on the sign of $\mathcal{D}(c(\varepsilon), y)$, we introduce the equidistant "chain" of points

$$\begin{cases} x_0 = c(\varepsilon), \;\; x_1 = c(0), \;\; x_2 = c(-\varepsilon), \;\ldots\; , x_k = c(-(k-1)\varepsilon) & \text{if } \mathcal{D}(c(\varepsilon), y) > 0 \\ x_0 = c(-\varepsilon), \;\; x_1 = c(0), \;\; x_2 = c(\varepsilon), \;\ldots\; , x_k = c((k-1)\varepsilon) & \text{if } \mathcal{D}(c(\varepsilon), y) < 0. \end{cases} \tag{6.5.25}$$

(Thus $y$ has timelike separation from $x_0$, lightlike separation from $x_1 = x$, and spacelike separation from $x_2, \ldots, x_k$). Then by construction, $x_0 \in \mathcal{I}(y)$, whereas all the other points of the chain are spacelike or lightlike separated from $y$.

For the proof of Theorem 6.19, it suffices to consider a chain of three points.

**Lemma 6.26.** *Assume that $\mathcal{D}(x, y)$ is symmetric (6.1.1) and equal to one on the diagonal, $\mathcal{D}(x, x) \equiv 1$. Then for $x_0, x_1, x_2$ as given by (6.5.25) in the case $k = 2$, there is a real constant $a_1$ such that for all sufficiently small $\varepsilon$,*

$$\mathcal{D}(x_i, x_j) = 1 + a_1\, |i - j|^2\, \varepsilon^2 + \mathcal{O}(\varepsilon^3) \qquad \textit{for all } i, j \in \{0, 1, 2\}\,. \tag{6.5.26}$$

*Proof.* We set $f(t, t') = \mathcal{D}(c(t), c(t'))$ for $t, t' \in (-2\varepsilon, 2\varepsilon)$. Using that $\mathcal{D}$ is symmetric and that $\mathcal{D}(x, x) \equiv 1$, we know hat

$$0 = \frac{d}{dt} f(t_0, t_0) = 2\, \frac{d}{dt} f(t_0, t)\big|_{t=t_0}\,.$$

Thus the linear term in a Taylor expansion vanishes,

$$f(t_0, t) = 1 + \frac{1}{2}\, g(t_0)\, (t - t_0)^2 + \mathcal{O}\big(|t - t_0|^3\big)\,,$$

where we set

$$g(t_0) = \frac{d^2}{dt^2} f(t_0, t)\Big|_{t=t_0}\,.$$

As the function $g$ is smooth, we can again expand it in a Taylor series,

$$g(t_0) = g(0) + \mathcal{O}(t_0)\,.$$

We thus obtain

$$f(t_0, t) = 1 + \frac{1}{2}\, g(0)\, (t - t_0)^2 + \mathcal{O}\big(|t_0|\, |t - t_0|^2\big) + \mathcal{O}\big(|t - t_0|^3\big)\,.$$

Setting $a_1 = 2g(0)$ and using that $|t|, |t_0| \leq 2\varepsilon$, the result follows. □

**Lemma 6.27.** *Under the assumptions of Theorem 6.19, statement* (6.5.24) *holds.*

*Proof.* Assume conversely that for $x \in \overset{\circ}{\operatorname{supp}}\, \rho$ there is a point $y \in \operatorname{supp} \rho \cap \mathcal{K}(x)$. We choose the chain $x_0, x_1 = x, x_2$ as in Lemma 6.26. We use the notation of Corollary 6.9 in case $N = 3$, setting $x_3 = y$. Choosing the vector $u \in \mathbb{C}^4$ as $u = (1, -2, 1, 0)$, we can apply Lemma 6.26 to obtain

$$\langle u, Lu \rangle_{\mathbb{C}^4} = 6 - 4\,\mathcal{D}(x_0, x_1) + 2\,\mathcal{D}(x_0, x_2) - 4\,\mathcal{D}(x_1, x_2) = \mathcal{O}(\varepsilon^3)\,.$$

Furthermore, using (6.5.17), we know that

$$\mathcal{D}(x_0, y) = b\,\varepsilon + \mathcal{O}(\varepsilon^2)$$

with $b \neq 0$. Thus, choosing $u = (\alpha, -2\alpha, \alpha, \beta)$ with $\alpha, \beta \in \mathbb{R}$, it is

$$\langle u, Lu \rangle_{\mathbb{C}^4} = \left\langle \begin{pmatrix} \alpha \\ \beta \end{pmatrix}, \begin{pmatrix} \mathcal{O}(\varepsilon^3) & b\varepsilon + \mathcal{O}(\varepsilon^2) \\ b\varepsilon + \mathcal{O}(\varepsilon^2) & 1 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \right\rangle_{\mathbb{C}^2}.$$

For sufficiently small $\varepsilon$, the matrix in this equation has a negative determinant, in contradiction to Corollary 6.9. □

This completes the proof of Theorem 6.19.

In order to finish the proof of Theorem 6.21, we first remark that combining the symmetry of $\mathcal{D}$ with the assumption that $\mathcal{D}$ is locally translation symmetric at $x$ with respect to $c$, we know that $\mathcal{D}(c(t), c(t')) = f(|t - t'|)$. After rescaling, we can assume that $f(0) = 1$. A Taylor expansion of $f$ then yields the following simplification and generalization of Lemma 6.26,

$$\mathcal{D}(c(t), c(t')) = 1 + \sum_{i=1}^{K} a_i\,(t - t')^{2i} + \mathcal{O}\Big((t - t')^{2(K+1)}\Big), \tag{6.5.27}$$

where the real coefficients $a_i$ only depend on $c$.

**Lemma 6.28.** *Under the assumptions of Theorem 6.21, the statement* (6.5.24) *holds.*

*Proof.* Let us first verify that in the real analytic case, there is a $p$ such that (6.5.19) holds. Namely, assuming the contrary, all the $t$-derivatives of the function $\mathcal{D}(c(t), y)$ vanish. As the function $\mathcal{D}(c(t), y)$ is real analytic in a neighborhood of $t = 0$ (as the composition of analytic functions is analytic), it follows that this function is locally constant. This contradicts the fact that $\mathcal{D}(c(t), y)$ changes sign at $t = 0$.

Assume conversely that for $x \in \overset{\circ}{\operatorname{supp}}\, \rho$ there is a point $y \in \operatorname{supp} \rho \cap \mathcal{K}(x)$. We choose the chain $x_0, x_1 = x, x_2, \ldots, x_k$ as in (6.5.25) with $k = p + 1$. We use the notation of Corollary 6.9 in case $N = k$. Then the Gram matrix $L$ becomes

$$L = \big(f(\varepsilon|i - j|)\big)_{i,j=0,\ldots,k} = \begin{pmatrix} 1 & f(\varepsilon) & \cdots & f(k\varepsilon) \\ f(\varepsilon) & 1 & & \\ \vdots & & \ddots & \\ f(k\varepsilon) & \cdots & & 1 \end{pmatrix}.$$

Using the expansion (6.5.27) for $K = k-1$, we obtain

$$\begin{aligned} L = E + a_1\varepsilon^2\big(|i-j|^2\big) + a_2\varepsilon^4\big(|i-j|^4\big) \\ + \ldots + a_{k-1}\varepsilon^{2(k-1)}\big(|i-j|^{2(k-1)}\big) + \mathcal{O}\big(\varepsilon^{2k}\big)\,, \end{aligned} \tag{6.5.28}$$

where $E$ denotes the matrix where all the matrix entries (also the off-diagonal entries) are equal to one, and $(|i-j|^q)$ is the matrix whose element $(i,j)$ has the value $|i-j|^q$.

Let us construct a vector $v \in \mathbb{C}^{k+1}$ such that the expectation value $\langle v, Lv\rangle$ is $\mathcal{O}(\varepsilon^{2k})$. To this end, we take for $v = (v_i)_{i=0}^k \in \mathbb{C}^{k+1}$ a non-trivial solution of the $k$ linear equations

$$\sum_{i=0}^k v_i = 0, \quad \sum_{i=0}^k i v_i = 0, \quad \sum_{i=0}^k i^2 v_i = 0, \quad \ldots, \sum_{i=0}^k i^{k-1} v_i = 0\,. \tag{6.5.29}$$

Then $\langle v, Ev\rangle = 0$ and for all $l \in \{1, \ldots, k-1\}$

$$\begin{aligned} \langle v, (|i-j|^{2l})v\rangle &= \sum_{i,j=0}^k v_i v_j |i-j|^{2l} = \sum_{i,j=0}^k v_i v_j \sum_{\nu=0}^{2l} \binom{2l}{\nu} i^\nu j^{2l-\nu} = \\ &= \sum_{i,j=1}^k v_i v_j \left( i^{2l} + 2l\; i^{2l-1} j + \ldots + \binom{2l}{l} i^l j^l + \ldots + j^{2l} \right). \end{aligned}$$

Each summand involves a power of $i$ and a power of $j$, where always one of these powers is smaller than $k$. Thus all summands vanish according to (6.5.29). The solution $v$ can always be normalized by $v_0 = 1$, because setting $v_0$ to zero, the system of equations (6.5.29) can be rewritten with the square Vandermonde matrix which has a trivial kernel. In view of the expansion (6.5.28), we conclude that $\langle v, Lv\rangle = \mathcal{O}(\varepsilon^{2k})$.

We next consider the setting of Corollary 6.9 in case $N = k+1$ and $x_{k+1} = y$. Using (6.5.19) together with the fact that the points $y$ and $x_0$ are timelike separated, we find that

$$\mathcal{L}(x_0, y) = b\,\varepsilon^p + \mathcal{O}(\varepsilon^{p+1}) \tag{6.5.30}$$

for $b \neq 0$. We choose the vector $u \in \mathbb{C}^{k+2}$ as $u = (\alpha v_0, \ldots, \alpha v_k, \beta)$ with $\alpha, \beta \in \mathbb{R}$,

$$\langle u, Lu\rangle_{\mathbb{C}^{k+2}} = \left\langle \begin{pmatrix} \alpha \\ \beta \end{pmatrix}, \begin{pmatrix} \mathcal{O}(\varepsilon^{2k}) & b\varepsilon^p + \mathcal{O}(\varepsilon^{p+1}) \\ b\varepsilon^p + \mathcal{O}(\varepsilon^{p+1}) & \mathcal{D}(y,y) \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \right\rangle_{\mathbb{C}^2},$$

where we combined (6.5.30) with our normalization $v_0 = 1$, and used that $y$ is not timelike separated from $x_1, \ldots, x_k$. For sufficiently small $\varepsilon$, the matrix in this equation has a negative determinant, in contradiction to Corollary 6.9. □

This completes the proof of Theorem 6.21.

The expansion (6.5.27) of the function $\mathcal{D}$ can be used to deduce more detailed informations on the support of the minimizing measure, as done in the following Corollary:

**Corollary 6.29.** *If the coefficients $a_1$, $a_2$ of (6.5.27) satisfy*

$$a_1 \geq 0 \quad \text{or} \quad 6a_2 - a_1^2 \leq 0, \tag{6.5.31}$$

*then there cannot exist a submanifold $U \subset \text{supp } \rho$ with $\dim(U) \geq 1$.*

*Proof.* Assume $U \subset \text{supp } \rho$ with $\dim(U) \geq 1$. For an $\varepsilon$-chain $x_0, x_1, x_2$ of timelike-separated points in $U$, the corresponding Gramian $L$ is given by

$$L = \begin{pmatrix} 1 & f(\varepsilon) & f(2\varepsilon) \\ f(\varepsilon) & 1 & f(\varepsilon) \\ f(2\varepsilon) & f(\varepsilon) & 1 \end{pmatrix}.$$

Using (6.5.27), the eigenvalues of $L$ are

$$-4a_1\varepsilon^2 + \mathcal{O}(\varepsilon^4), \quad \left(-\frac{2a_1^2}{3} + 4a_2\right)\varepsilon^4 + \mathcal{O}(\varepsilon^6), \quad 3 + \mathcal{O}(\varepsilon^2).$$

According to the conditions, the eigenvalues are negative, in contradiction to Corollary 6.9. □

We note that considering a Gramian corresponding to a larger number of points yields in a similar way conditions on higher coefficients.

We complete the Chapter with a remark on the support of the minimizing measure. According to the above Corollary, under certain conditions the support of the minimizing measure is singular in the sense that there cannot exist three points which are too closely neighbored. If the minimizing measure is additionally generically timelike, we can also use Proposition 6.18 and see that the support of the minimizing measure cannot be concentrated at a subset but must be spread out. An accurate characterization of the support of the minimizing measure is still outstanding.

# 7 Applications of the Structural Results to the Circle and the Sphere

## 7.1 The Variational Principles on the Circle

We will now apply the general structural results on basic examples. As a simple starting point for a more detailed analysis, we now consider the variational principle (5.6.21) on weighted counting measure (5.5.18) restricted on the circle $S^1$, where the action is defined via the argument function $\mathcal{D}$ given by (5.1.10) restricted on $S^1 \times S^1$. Applying the general structural results, we will prove the transition between generically timelike and singular measures and show that under generic assumptions the singular minimizing measure is supported at only a finite number of points. Moreover, we will give many minimizers in closed form.

The numerical solution methods and results are similar to those on $S^2$. As starting configuration, we choose in analogy of the Tammes distribution on $S^2$ a uniform distribution of $m$ points on the circle,

$$X_m = \{x_k = e^{i(k-1)\vartheta_m} \;:\; k = 1, \ldots, m\}\,, \qquad \vartheta_m = \frac{2\pi}{m}\,, \tag{7.1.1}$$

with uniform weights $\rho_k = 1/m$. Minimizing with the simulated annealing algorithm discussed in 5.3, we obtain the result shown in Figure 7.1. The numerical results indicate that the minimizing measure is supported at a finite number of points $m_0$.

This number can be stated explicitly by

$$m_0 = \min \left\{ n \in \mathbb{N} \;:\; n \geq \frac{2\pi}{\vartheta_{\max}} \right\}\,, \tag{7.1.2}$$

where $\vartheta_{\max}$ given by (5.1.11) denotes the opening angle of the light-cone. The number $m_0$ increases with $\tau$, with discontinuous "jumps" at the values

$$\tau_m := \sqrt{\frac{2}{1 - \cos(\vartheta_m)}}, \tag{7.1.3}$$

in analogy to (5.2.13). Besides the discrete nature of the minimizers, the numerical results reveal that at $\tau = \tau_c = \sqrt{2}$ (corresponding to $\vartheta_{\max} = \frac{\pi}{2}$), the structure of the minimizers changes completely. Just as in Section 5.6, this effect can be understood as a phase transition. More precisely, if $\tau \leq \tau_c$, every minimizer is generically

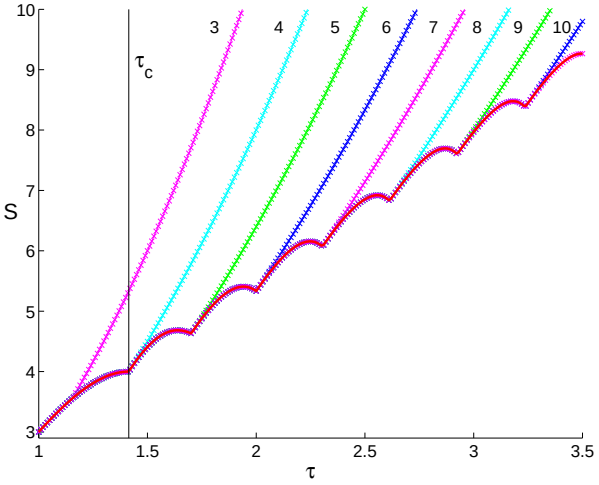



Figure 7.1: Numerical minima for the weighted counting measure on the circle.

timelike. If we further decrease $\tau$ (i.e.. for every fixed $1 \leq \tau < \tau_3$), we even found a large number of minimizing measures, supported at different numbers of points with strikingly different positions. If $\tau > \sqrt{2}$, the minimizer is unique (up to rotations on $S^1$), is supported at $m_0$ points, and is not generically timelike.

We exemplarily explain these features in the case $m = 10$ and illustrate them by regarding the plots of the functions $\ell$ and $\mathsf{d}$ depending on $\vartheta$, see Figure 7.2:

- For $1 \leq \tau < \tau_3$, there are many different generically timelike minimizers with a different number of points in the support. In the case $\tau = 1$ it is $\mathsf{d} \equiv \ell \equiv \mathcal{S}$ else $\mathsf{d} \leq \ell$ If $\tau < 2\sqrt{\frac{2}{5+\sqrt{5}}}$, the starting point $X_{10}$ with equal weighting factors is a generically timelike minimizer.

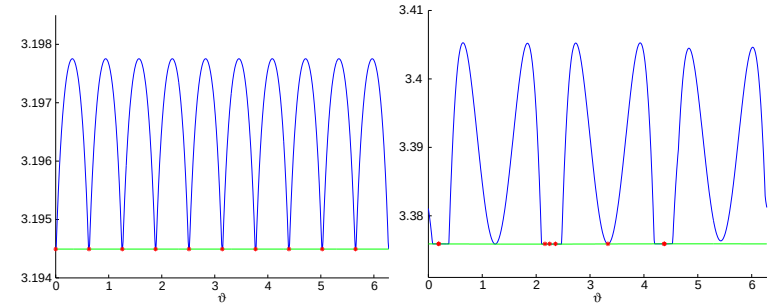
- For $\tau \in (\tau_3, \tau_4]$, the measure supported at $X_4$ seems the unique minimizer, which is generically timelike.

- For $\tau > \sqrt{2} = \tau_4$, the minimizing measure is only supported on few points, but there exists no generically timelike minimizer.

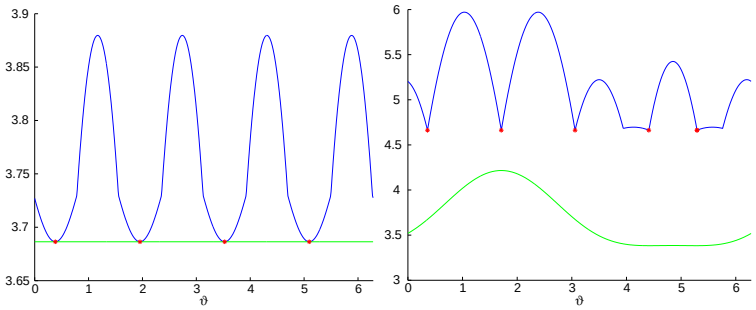
- For $\tau > \tau_{10} \approx 3.23607$ the Euler-Lagrange-equations are violated, and we conclude that there cannot exist a minimizer supported at less than 11 points.

In the remainder of this section, we make this picture rigorous. Since the function $\mathcal{D}$ is U(1)-invariant, the standard normalized volume measure on the circle is a homogenizer of the function $\mathcal{D}$. The operator $\mathcal{D}_\mu$ can be diagonalized explicitly by plane waves $\phi_n(x) = e^{in\vartheta_x}$ (where $n \in \mathbb{Z}$, and $\vartheta_x$ is the angle). This gives rise to the decomposition

$$\mathcal{D}(x,y) = \nu_0 + \sum_{n=1}^{2} \nu_n \left( e^{in(\vartheta_x - \vartheta_y)} + e^{-in(\vartheta_x - \vartheta_y)} \right),$$




(a) $\tau = 1.05$ (b) $\tau = 1.1$




(c) $\tau = 1.2$ (d) $\tau = 1.6$

Figure 7.2: The functions $\mathsf{d}$ (green) and $\ell$ (blue) depending on $\vartheta$ together with the points in the support of the minimizing measure $\rho$ (red) and different values of $\tau$.

where

$$\nu_0 = \iint_{S^1 \times S^1} \mathcal{D}(x,y)\, d\mu(x)\, d\mu(y) = 4\tau^2 - \tau^4 \,. \tag{7.1.4}$$

and similarly $\nu_1 = 2\tau^2$ and $\nu_2 = \frac{1}{2}\tau^4$. In the case $\tau \leq 2$ all eigenvalues $\nu_0$, $\nu_1$ and $\nu_2$ are non-negative, and we can apply Proposition 6.15 to obtain

$$\mathcal{S}_{\min} \geq \nu_0 \,.$$

For sufficiently small $\tau$, the uniform distribution of points on the circle (7.1.1) gives a family of generically timelike minimizers.

**Lemma 7.1.** *If $m \geq 3$ and $\tau$ is so small that $\mathcal{L}(x,y) = \mathcal{D}(x,y)$ for all $x, y \in X_m$, then $\rho = \frac{1}{m}\sum_{i=1}^m \delta_{x_i}$ is a generically timelike minimizer. Every other minimizer is also generically timelike.*

*Proof.* A straightforward calculation using the identities

$$\sum_{k=0}^{m-1} e^{ik\vartheta_m} = 0 \qquad \text{and} \qquad \sum_{k=0}^{m-1} \left(e^{ik\vartheta_m}\right)^2 = 0$$

yields for any $x \in S^1$

$$\begin{aligned}\mathsf{d}(x) &= \frac{1}{m} 2\tau^2 \sum_{k=0}^{m-1} \big(2 + 2\langle x, x_k\rangle - \tau^2 + \tau^2 \langle x, x_k\rangle^2\big) \\ &= \frac{1}{m} 2\tau^2 \Big(2m - m\tau^2 + \frac{m}{2}\,\tau^2\Big) = \nu_0\,.\end{aligned}$$

In particular, one sees that $\mathcal{S}[\rho] = \nu_0$.

The assumption $\mathcal{L}(x,y) = \mathcal{D}(x,y)$ for all $x, y \in X_m$ can only be satisfied if $\tau < 2$. Thus in view of (7.1.4), the operator $D_\mu$ is positive semi-definite. We finally apply Proposition 6.15. □

Applying this lemma in the case $m = 4$ gives the following result.

**Corollary 7.2.** *If $\tau \le \tau_c$, every minimizer is generically timelike.*

More general classes of generically timelike minimizers can be constructed explicitly with the help of Corollary 6.16. In particular, one can find minimizing measures which are not discrete. For the details we refer to the analogous measure on $S^2$ given in Example 7.10.

Having explored the case $\tau \le \tau_c$, we proceed with the case $\tau > \tau_c$. As already stated, the closed light-cones are given by

$$\mathcal{J}(x) = \Big\{ y \;:\; x \cdot y \geq 1 - \frac{2}{\tau^2} = \cos(\vartheta_{\max}) \Big\} \cup \{-x\}\,.$$

Therefore if $\tau > \sqrt{2} = \tau_c$ (or equivalently $\vartheta_{\max} < \frac{\pi}{2}$), the condition of antipodal points (see Proposition 6.17) is satisfied. Thus there are no generically timelike minimizers. As the condition (6.5.17) is obvious, we can apply Theorem 6.19 (A) and conclude that

$$\text{if } \tau > \tau_c, \text{ every minimizing measure is discrete}\,. \tag{7.1.5}$$

Using results and methods from Section 6.5, we we will be able to explicitly construct all minimizers under the additional technical assumption that

$$\tau > \tau_d := \sqrt{3 + \sqrt{10}}\,.$$

We first introduce a descriptive notation:

**Definition 7.3.** *A **chain** of length $k$ is a sequence $x_1, \ldots, x_k \in S^1$ of pairwise distinct points such that $x_i \cdot x_{i+1} = \cos(\vartheta_{\max})$ for all $i = 1, \ldots, k-1$.*

**Theorem 7.4.** *If $\tau > \tau_d$, the support of every minimizer $\rho$ is a chain $\{x_1, \ldots, x_{m_0}\}$ (with $m_0$ as given by (7.1.2)). The minimal action is*

$$\mathcal{S}_{\min} = \frac{\mathcal{L}(0)(\mathcal{L}(0) + \mathcal{L}(\gamma))}{(m_0 - 2)(\mathcal{L}(0) + \mathcal{L}(\gamma)) + 2\mathcal{L}(0)}\,, \tag{7.1.6}$$

*where $\gamma = \arccos(x_1 \cdot x_{m_0}) \in (0, \vartheta_{\max}]$. The minimizing measure is unique up to rotations on $S^1$.*

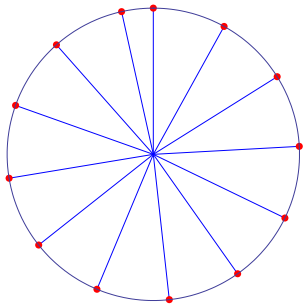


Figure 7.3: A minimizer for $\tau = 4$.

An example for the support of the minimizing measure is shown in Figure 7.3. Up to rotations, the points of the chain can be written as

$$x_k = e^{i(k-1)\vartheta_{\max}}, \quad k = 1, \ldots, m_0. \tag{7.1.7}$$

In the special cases $\tau = \tau_m$, the minimizer is the measure with equal weights supported on the uniform distribution $X_m$. In the general case, the weights will not all be the same, as will be specified below.

For the proof of Theorem 7.4 we proceed in several steps.

**Lemma 7.5.** *If $\tau > \sqrt{6}$, the minimal action is attained for a measure supported on a chain $x_1, \ldots, x_k$. In the case $k = m_0$, every minimizing measure is a chain.*

*Proof.* Let $\rho$ be a minimizing measure. We first note that every chain $K$ in the support of $\rho$ must have finite length, because otherwise $\vartheta_{\max}/\pi$ would have to be irrational. As a consequence, $K$ would be a dense set of $S^1$, in contradiction to the discreteness of $\rho$ (see (7.1.5)). Let us assume that the support of $\rho$ is not a chain.

We let $K \subset \operatorname{supp} \rho$ be a chain, which is maximal in the sense that it cannot be extended. Set $L = \operatorname{supp} \rho \setminus K$. We consider variations of $\rho$ where we rotate $K$ by a small angle $\vartheta$, leaving the weights on $K$ as well as $\rho|_L$ unchanged. The fact that $K$ cannot be extended implies that that these variations are smooth in $\vartheta$ at $\vartheta = 0$. The minimality of $\rho$ implies that

$$\delta \mathcal{S} = 0 \quad \text{and} \quad \delta^2 \mathcal{S} = \sum_{x \in K, y \in L} 2\, \rho(x)\, \rho(y)\, \delta^2 \mathcal{L}(x,y) \geq 0\,. \tag{7.1.8}$$

On the other hand, differentiating (5.1.10), one finds that the function $\mathcal{D}$ restricted to $[0, \vartheta_{\max}]$ is concave,

$$\mathcal{D}''(\vartheta) = -4\tau^2(\cos(\vartheta) + \tau^2 \cos(2\vartheta)) < 0 \qquad (\text{if } \tau > \sqrt{6})\,. \tag{7.1.9}$$

Comparing with (7.1.8), we conclude that $\mathcal{L}(x,y)$ vanishes for all $x \in K$ and $y \in L$. In the case that $\# K = m_0$, this implies that $L = \varnothing$, a contradiction. In the remaining case $\# K < m_0$, we can subdivide the circle into two disjoint arcs $A_K$ and $A_L$ such that $K \subset A_K$ and $L \subset A_L$. The opening angle of $A_K$ can be chosen larger than $\vartheta_{\max}$ times the length of $K$, giving an a-priori upper bound on the length of $K$.

By further rotating $K$, we can arrange that the chain $K$ can be extended by a point in $L$, without changing the action. If the extended chain equals the support of $\rho$, the proof is finished. Otherwise, we repeat the above argument with $K$ replaced by its extension. In view of our a-priori bound on the length of $K$, this process ends after a finite number of steps. □

**Lemma 7.6.** *Suppose that $\rho$ is a minimizing measure supported on a chain. If $\tau > \sqrt{3+\sqrt{10}}$, the length of this chain is at most $m_0$.*

*Proof.* For all $\gamma \in (0, \vartheta_{\max})$ an elementary calculation shows that

$$\mathcal{L}(\gamma)^2 + \mathcal{L}(\vartheta_{\max} - \gamma)^2 > \mathcal{L}(0)^2. \tag{7.1.10}$$

In the case $\tau = \tau_{m_0}$ there is nothing to prove. Thus we can assume that $\tau \neq \tau_{m_0}$. For a chain $x_1, \ldots, x_k$ with $k > m_0$, the Gram matrix corresponding to the points $x_1, x_{m_0+1}, x_2$ has the form

$$\begin{pmatrix} \mathcal{L}(0) & \mathcal{L}(\vartheta_{\max}-\gamma) & 0 \\ \mathcal{L}(\vartheta_{\max}-\gamma) & \mathcal{L}(0) & \mathcal{L}(\gamma) \\ 0 & \mathcal{L}(\gamma) & \mathcal{L}(0) \end{pmatrix}. \tag{7.1.11}$$

Using (7.1.10), its determinant is negative, in contradiction to Corollary 6.9. □

From the last two lemmas we conclude that every minimizer $\rho$ is supported on one chain of length at most $m_0$. Parameterizing the points as in (7.1.7), the only contributions to the action come from $\mathcal{L}(x_l, x_l)$ and $\mathcal{L}(x_1, x_{m_0})$. Using Lagrange multipliers, the optimal weights $\rho_i = \rho(x_i)$ are calculated to be

$$\rho_1 = \rho_{m_0} = \frac{\lambda}{\mathcal{L}(0)+\mathcal{L}(\gamma)} \qquad \text{and} \qquad \rho_i = \frac{\lambda}{\mathcal{L}(0)} \quad \text{for } i = 2, \ldots, m_0 - 1\,, \tag{7.1.12}$$

where we set

$$\lambda = \frac{\mathcal{L}(0)\,(\mathcal{L}(0)+\mathcal{L}(\gamma))}{(m_0-2)(\mathcal{L}(0)+\mathcal{L}(\gamma)) + 2\mathcal{L}(0)}\,.$$

The corresponding action is computed to be $\mathcal{S}[\rho] = \lambda$, giving the formula in (7.1.6). Using this explicit value of the action, we obtain the following

**Lemma 7.7.** *Suppose that $\rho$ is a minimizing measure supported on a chain. Then the length of this chain is at least $m_0$.*

*Proof.* For a chain of length $n < m_0$, the only contribution to the action come from $\mathcal{L}(x_l, x_l)$, $l = 1, \ldots, n$. The corresponding optimal weights are computed by $\rho_i = 1/n$. The resulting action is

$$\mathcal{S} = \sum_{i=1}^{n} \frac{1}{n^2} \mathcal{L}(x_i, x_i) = \frac{1}{n} \mathcal{L}(0)\,.$$

This is easily verified to be strictly larger than the value of the action in (7.1.6). □

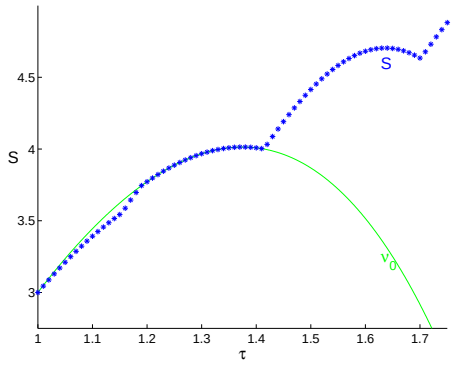



Figure 7.4: The numerical minimum and the value $\nu_0$ for the function $\mathcal{B}$.

This completes the proof of Theorem 7.4.

We finally remark that if $\tau$ lies in the interval $(\sqrt{2}, \sqrt{3+\sqrt{10}})$ where Theorem 7.4 does not apply, the numerics show that the minimizing $\rho$ is again the measure supported on the chain of length $m_0$, with one exception: If $\tau$ is in the interval $(1.61988, \tau_5)$ with $\tau_5 = \sqrt{2+\frac{2}{\sqrt{5}}}$, a chain of length $m_0+1 = 6$ gives a lower action than the chain of length 5. In this case, the Gram matrix (7.1.11) is indeed positive definite, so that the argument in Lemma 7.7 fails.

The existence of generically timelike minimizers is in general hard to prove, even in the case that the underlying manifold is the circle. Estimating the action by the eigenvalue $\nu_0$, the property $\mathcal{D}_\mu \geq 0$ is essential. If it fails, the eigenvalue can no longer be used as an estimate neither from above nor below, as the following example shows:

*Example* 7.8. Let $\mathcal{B} : S^1 \times S^1 \to \mathbb{R}$ depending on the angle between two points given by

$$\mathcal{B}(\vartheta) = \frac{1}{\tau^2}(1+\cos\vartheta)\left(2-(1-\cos\vartheta)\tau^2\right)\left(\cos\vartheta - 1 + (1-\cos\vartheta)\tau^2 + 2\tau^4\right).$$

Then $\mathcal{B}$ coincides with the function $\mathcal{D}$ for $\tau = 1$. For $\tau > 1$, it is $\mathcal{B}(0) = 8\tau^2$, $\mathcal{B}(\pi) = 0$ and $\mathcal{B}$ changes sign at $\vartheta_{\max}$, thus the light-cones coincide with the light-cones corresponding to $\mathcal{D}$. Although the two functions look quite similar, the estimate with the eigenvalue corresponding to the constant function, now given as

$$\nu_0 = \frac{1}{2\tau^2}(-2+3\tau^2+7\tau^4-2\tau^6)$$

fails, see picture 7.4. If $\tau$ is close to one, the measure supported at the points $X_3$ with equal weights is a minimizing measure whose action is less than $\nu_0$ and which is not generically timelike. If $\tau \gg \tau_3$, the measure supported at the points $X_4$ with equal weights is a generically timelike minimizer. If $\tau > \sqrt{2}$, the minimizing measures build chains, like in the example above. ◊

## 7.2 The Analysis of the Variational Principle on the Sphere

We now attend on the analysis of the variational principles on the sphere (see Chapter 5). Applying Theorem 6.19 (A) with the curve $c$ chosen as the grand circle joining $x$ and $y$, we immediately obtain that every minimizing measure $\rho$ on $S^2$ is either generically timelike or $\overset{\circ}{\operatorname{supp}}\rho = \varnothing$. The numerics in Section 5.6 indicated that these two cases are separated by a "phase transition" at $\tau = \tau_c = \sqrt{2}$. We will now prove that this phase transition really occurs. Moreover, we will develop methods for estimating the minimal action from above and below.

### 7.2.1 Generically Timelike Minimizers

As the function $\mathcal{D}$ is U(2)-invariant, the standard normalized volume measure on the sphere is a homogenizer of the function $\mathcal{D}$. We first decompose $\mathcal{D}$ in spherical harmonics. A short calculation yields in analogy to (6.4.13) the decomposition

$$\mathcal{D}(x,y) = \nu_0 + 4\pi \sum_{l=1}^{2} \nu_l \sum_{m=-l}^{l} Y_l^m(x)\overline{Y_l^m(y)}\,,$$

where the eigenvalues are given by

$$\nu_0 = 4\,\tau^2 - \frac{4}{3}\,\tau^4\,, \qquad \nu_1 = \frac{4}{3}\,\tau^2\,, \qquad \nu_2 = \frac{4}{15}\,\tau^4\,. \tag{7.2.13}$$

In particular, the operator $\mathcal{D}_\mu$ is positive semi-definite if $\tau \leq \sqrt{3}$.

If $\tau \leq \tau_c$, there is a large family of minimizers, as we now discuss. The simplest example is the measure supported on the octahedron $X_6$, defined in (5.4.17), with equal weights $\frac{1}{6}$. Obviously, the condition (i) in Definition 6.11 is satisfied. Moreover, for any $x \in S^2$ one calculates

$$\begin{aligned}\mathsf{d}(x) &= \frac{1}{6} \sum_{y \in \operatorname{supp}\rho} 2\tau^2 \left(2 + 2x\cdot y - \tau^2 + \tau^2 (x\cdot y)^2\right) \\ &= \frac{1}{3}\tau^2 \left(12 - 6\tau^2 + 2\tau^2(x_1^2 + x_2^2 + x_3^2)\right) = \nu_0\,.\end{aligned}$$

Thus Proposition 6.15 yields that $\rho$ is a generically timelike minimizer. Moreover, from Proposition 6.15 we conclude that every minimizer is generically timelike. If conversely $\tau > \tau_c$, the condition of antipodal points is fulfilled, and thus Proposition 6.17 shows that no generically timelike minimizers exist. We have thus proved the following result.

**Corollary 7.9.** *If $\tau \leq \tau_c$, every minimizing measure $\rho$ on $S^2$ is generically timelike, and the minimal action is equal to $\nu_0$ as given by (7.2.13). If conversely $\tau > \tau_c$, every minimizing measure $\rho$ is not generically timelike and $\overset{\circ}{\operatorname{supp}}\rho = \varnothing$.*

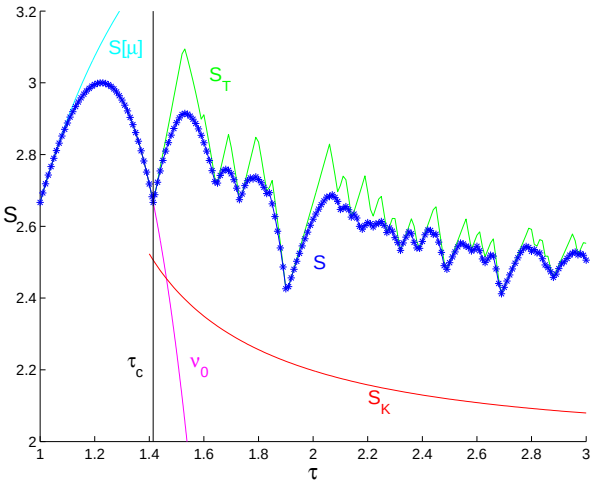



Figure 7.5: Estimates of the action on $S^2$: Upper bounds obtained from the volume measure $S[\mu]$ and from the Tammes distribution $S_T$, lower bounds by $\nu_0$ and by the heat kernel estimate $S_K$.

Similarly, one can show that if $\tau \leq \sqrt{\frac{3}{2}}$, the equal weighted measure supported at the tetrahedron is another example for a generically timelike minimizer. Using Corollary 6.16, for small $\tau$ one can also construct minimizers which are not discrete, as is illustrated by the following example.

*Example* 7.10. *We introduce the function* $f \in L^2(S^2)$ *by*

$$f(\vartheta,\varphi) = \begin{cases} \frac{5}{3} & \text{if } \vartheta \in [0, \arccos(0.8)], \\ \frac{35}{9} & \text{if } \vartheta \in [\arccos(0.4), \arccos(0.2)] \\ \frac{40}{9} & \text{if } \vartheta \in [\arccos(-0.5), \arccos(-0.7)], \\ 0 & \text{otherwise.} \end{cases}$$

*Then if* $\tau < 1.00157$, *a straightforward calculation shows that* $f$ *has the properties (a) and (b) of Corollary 6.16. Thus the measure* $d\rho = f d\mu$ *is a minimizing generically timelike measure with* $\overset{\circ}{\operatorname{supp}}\, \rho \neq \varnothing$. ◊

## 7.2.2 Estimates of the Action

As not even the solution of the Tammes problem is explicitly known, we cannot expect to find explicit minimizers for general $\tau$. Therefore, we need good estimates of the action from above and below. We now explain different methods for getting estimates, which are all compiled in Figure 7.5.

Estimates from above can be obtained simply by computing the action for suitable test measures. For example, the action of the normalized volume measure is

$$\mathcal{S}[\mu] = \frac{1}{4\pi} \int_0^{2\pi} d\varphi \int_0^{\vartheta_{\max}} d\vartheta \, \sin\vartheta \, \mathcal{D}(\vartheta) = 4 - \frac{4}{3\tau^2} \geq \mathcal{S}_{\min} \,.$$

As one sees in Figure 7.5, this estimate is good if $\tau$ is close to one. Another example is to take the measure supported at the Tammes distribution for $K$ points, with equal weights. We denote the corresponding action by $\mathcal{S}_T^K$. We then obtain the estimate

$$\mathcal{S}_{\min} \leq \mathcal{S}_T := \min_K \mathcal{S}_T^K \,.$$

One method is to compute $\mathcal{S}_T$ numerically using the tables in [28]. This gives quite good results (see Figure 7.5), with the obvious disadvantage that the estimate is not given in closed form. Moreover, the Tammes distribution, see 5.2, is useful for analyzing the asymptotics for large $\tau$. For given $\tau > 1$ we choose $K \in \mathbb{N}$ such that $\tau_{K-1} \leq \tau < \tau_K$. Then using the estimate (5.2.14) we obtain

$$\mathcal{S}_{\min} \leq \mathcal{S}_T^{K-1} = \frac{8\tau^2}{K-1} < \frac{8\tau_K^2}{K-1} \leq 32\,\frac{K}{K-1}\left(\left(\frac{8\pi}{\sqrt{3}}\right)^{1/2} - \frac{C}{K^{1/6}}\right)^{-2}.$$

In the limit $\tau \to \infty$, we know that $K \to \infty$, and thus

$$\limsup_{\tau\to\infty} \mathcal{S}_{\min} \geq \frac{4\sqrt{3}}{\pi} \,.$$

Constructing a lower bound is more difficult. From (7.2.13) it is obvious that the operator $\mathcal{D}_\mu$ is positive semi-definite if $\tau \leq \sqrt{3}$. Thus we can apply Proposition 6.15 to obtain

$$\mathcal{S}_{\min} \geq \nu_0 \qquad \text{if } \tau \leq \sqrt{3}\,.$$

If $\tau \leq \sqrt{2}$, this lower bound is even equal to $\mathcal{S}_{\min}$ according to Corollary 7.9. As shown in Figure 7.5, the estimate is no longer optimal if $\tau > \sqrt{2}$.

Another method to obtain lower bounds is based on the following observation:

**Proposition 7.11.** *Assume that $K_\mu$ is an integral operator on $\mathcal{H}_\mu$ with integral kernel $K \in C^0(S^2 \times S^2, \mathbb{R})$ with the following properties:*

*(a) $K(x,y) \leq \mathcal{L}(x,y)$ for all $x, y \in S^2$.*

*(b) The operator $K_\mu$ is positive semi-definite.*

*Then the minimal action satisfies the estimate*

$$\mathcal{S}_{\min} \geq \iint_{S^2\times S^2} K(x,y)\, d\mu(x)\, d\mu(y)\,. \tag{7.2.14}$$

*Proof.* For any $\rho \in \mathfrak{M}$, assumption (a) gives rise to the estimate

$$\mathcal{S}[\rho] = \iint_{S^2\times S^2} \mathcal{L}(x,y) d\rho(x) d\rho(y) \geq \iint_{S^2\times S^2} K(x,y) d\rho(x) d\rho(y)\,.$$

Next, using property (b), we can apply Proposition 6.6 to conclude that the volume measure $\mu$ is a minimizer of the variational principle corresponding to $K$, i.e.

$$\iint_{S^2\times S^2} K(x,y)\, d\rho(x)\, d\rho(y) \geq \iint_{S^2\times S^2} K(x,y)\, d\mu(x)\, d\mu(y)\,.$$

Combining these inequalities gives the result. □

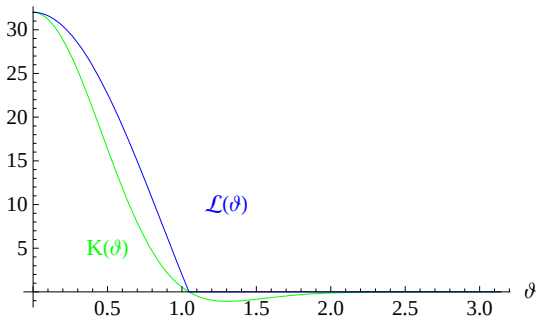



Figure 7.6: The Lagrangian $\mathcal{L}$ and the function $K$ in the heat kernel estimate for $\tau = 2$.

In order to construct a suitable kernel, we first consider the heat kernel $h_t$ on $S^2$,

$$h_t(x,y) = \left(e^{t\Delta_{S^2}}\right)(x,y) = 4\pi \sum_{l=0}^{\infty} e^{-t\,l(l+1)} \sum_{m=-l}^{l} Y_l^m(x)\overline{Y_l^m(y)}\,.$$

The heat kernel has the advantage that condition (b) is satisfied, but condition (a) is violated. This leads us to choosing $K$ as the difference of two heat kernels,

$$K(x,y) = \lambda \left(h_{t_1}(x,y) - \delta h_{t_2}(x,y)\right)\,. \tag{7.2.15}$$

For given $t_1 < t_2$, we choose $\delta$ and $\lambda$ such that $K(x,x) = 1$ and $K(\vartheta_{\max}) = 0$, i.e.

$$\delta = \frac{h_{t_1}(\vartheta_{\max})}{h_{t_2}(\vartheta_{\max})} < 1 \qquad \text{and} \qquad \lambda = \frac{\mathcal{L}(0)}{h_{t_1}(0) - \delta\, h_{t_2}(0)} > 0\,.$$

By direct inspection one verifies that condition (a) is satisfied (see Figure 7.6 for a typical example). The eigenvalues of the operator $K_\mu$ are computed to be

$$\lambda\left(e^{-t_1\,l(l+1)} - \delta\, e^{-t_2\,l(l+1)}\right),$$

showing that the operator $K_\mu$ is indeed positive semi-definite. Thus we can apply Proposition 7.11. Using that

$$\iint_{S^2\times S^2} h_t(x,y)\,d\mu(x)\,d\mu(y) = \iint_{S^2\times S^2} 4\pi\, Y_0^0(x)\overline{Y_0^0(y)}\,d\mu(x)\,d\mu(y) = 1\,,$$

we obtain the **heat kernel estimate**

$$\mathcal{S}_{\min} \geq S_K = \lambda\,(1-\delta)\,.$$

In this estimate, we are still free to choose the parameters $t_1$ and $t_2$. By adjusting these parameters, one gets the lower bound shown in Figure 7.5. Thus the heat kernel estimate differs from the minimal action only by an error of about 20%, and describes the qualitative dependence on $\tau$ quite well. But of course, it does not take into account the discreteness of the minimizers. We finally remark that for small $\vartheta$ the function $\mathcal{D}$ can be expanded as

$$\mathcal{D}(\vartheta) = 8\tau^2 - 2\vartheta^2\left(\tau^4+\tau^2\right) + \frac{1}{6}\vartheta^4\left(4\tau^4+\tau^2\right) + \mathcal{O}\left(\vartheta^6\right)$$

concluding that for $\tau > \sqrt{3+\sqrt{10}} = \tau_d$ Corollary 6.29 can be applied.

# 8 Causal Variational Principles on Flag Manifolds

## 8.1 Preliminaries

We now investigate the causal variational principles introduced in Section 2.2 on the space $\mathcal{F}$ of hermitian $f \times f$-matrices with prescribed eigenvalues $\alpha$ and $-\beta$ in higher dimension with regard to the structural results of Chapter 6. As mentioned in Section 3.2, this space can be identified with the flag manifold $\mathcal{F}_{1,2}(\mathbb{C}^f)$.

For the following calculations, we introduce the *Dirac delta function*

$$\delta : C_0^\infty(\mathbb{R}) \to \mathbb{R}, \quad f \mapsto f(0),$$

which may formally be written as $\int_{-\infty}^{\infty} f(x)\delta(x)dx = f(0)$. Using the *Heaviside function*

$$\Theta : \mathbb{R} \to \mathbb{R}, \quad \Theta(x) = \begin{cases} 0 & \text{if } x < 0 \\ \frac{1}{2} & \text{if } x = 0 \\ 1 & \text{if } x > 0, \end{cases}$$

the basic properties of the $\delta$-function (see [7, Chapter 2.3]) can be written as follows:

**Proposition 8.1.** *Let $g \in C_0^\infty(\mathbb{R})$ be a function with only a finite number of zeros $(x_i)_{i \in \mathcal{I}}$ which are all simple, and let $a \in \mathbb{R} \cup \{-\infty\}$. Then for all $f \in C_0^\infty(\mathbb{R})$ it is*

$$\int_a^\infty \delta\big(g(x)\big)\, f(x)dx = \sum_{i \in \mathcal{I}} \frac{f(x_i)}{|g'(x_i)|}\, \Theta(x_i - a). \tag{8.1.1}$$

In the case $a = -\infty$, the relation $\int_{-\infty}^{\infty} \delta\big(g(x)\big)\, f(x)dx = \sum_{i \in \mathcal{I}} \frac{f(x_i)}{|g'(x_i)|}$ generalizes the scaling property $\delta(\lambda x) = \frac{1}{|\lambda|}\delta(x)$ for $\lambda \in \mathbb{R}\backslash\{0\}$ to the composition with a function.

The delta function is similarly defined in higher dimensions as $\delta^n : C_0^\infty(\mathbb{R}^n) \to \mathbb{R}$ with $\delta^n(f) = f(0)$, formally written as $\delta^n(x) = \delta(x_1) \ldots \delta(x_n)$.

Using the basic properties, we can deduce special rules which we use in the following calculations. We will need the area of the $(n-1)-$sphere $S^{n-1} \subset \mathbb{R}^n$ for $n \in \mathbb{N}$, $n \geq 2$, which is given by

$$\text{vol}(S^{n-1}) = \frac{2\, \pi^{n/2}}{\Gamma(n/2)}, \tag{8.1.2}$$

where $\Gamma$ denotes the Gamma function.

**Lemma 8.2.** *For $n \in \mathbb{N}$, $n \geq 2$, let $\|.\|$ denote the standard Euclidean norm on $\mathbb{R}^n$. Then*

$$\int_{\mathbb{R}^n} \delta\big(\|x\|^2 - 1\big)\, dx = \frac{1}{2}\, \mathrm{vol}(S^{n-1}). \tag{8.1.3}$$

*Proof.* Since the integrand is radial symmetric, one obtains

$$\int_{\mathbb{R}^n} \delta\big(\|x\|^2 - 1\big)\, dx = \mathrm{vol}(S^{n-1}) \int_0^\infty dr\; r^{n-1}\, \delta(r^2 - 1),$$

where using formula (8.1.1) one calculates $\int_0^\infty dr\; r^{n-1}\delta(r^2-1) = \frac{1}{2}$. □

In the following calculations, additionally we use the *Beta function* which is given by

$$B(x,y) = \int_0^1 dt\; t^{x-1}(1-t)^{y-1} = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)} \quad \text{for} \quad x, y > 0. \tag{8.1.4}$$

## 8.2 Correlation Matrices of Rank One

We start the analysis with considering the case $\beta = 0$. In this case, $\mathcal{F}$ is the family of hermitian $f \times f$-matrices of rank one with non-vanishing eigenvalue $\alpha > 0$. An element $x$ in $\mathcal{F}$ can be represented as

$$x = \alpha |u)(u| \quad \text{for} \quad u \in \mathbb{C}^f \;\text{ with }\; \|u\| = 1, \tag{8.2.5}$$

where again $(.|.)$ denotes the standard Euclidean scalar product on $\mathbb{C}^f$ and $\|.\|$ the induced norm. The functions $\mathcal{L}$ and $\mathcal{D}$ on $\mathcal{F} \times \mathcal{F}$ defined in (2.4.30) coincide, and simplify to

$$\mathcal{D}(x,y) = \mathcal{L}(x,y) = \frac{1}{2}\, \mathrm{Tr}\big(xy\big)^2. \tag{8.2.6}$$

Since the function $\mathcal{D}$ is always non-negative, the causal structure defined in Definition 6.3 can be lightly stated: If $x, y \in \mathcal{F}$ are represented via (8.2.5) by vectors $u_x$ and $u_y$ in $\mathbb{C}^f$, the light-cones are $\mathcal{I}(x) = \{y \in \mathcal{F} \;:\; (u_x|u_y) \neq 0\}$, $\mathcal{J}(x) = \mathcal{F}$ and $\mathcal{K}(x) = \varnothing$.

With regard to Definition 6.5, the invariant normalized volume measure on the complex sphere is a homogenizer. Denoting by $du$ the Lebesgue measure on $\mathbb{C}^f$, the homogenizer $\mu \in \mathfrak{M}$ can be written as

$$d\mu = \frac{2}{\mathrm{vol}(S^{2f-1})}\; \delta(\|u\|^2 - 1) du, \tag{8.2.7}$$

where formula (8.1.3) proves the normalization. The corresponding integral operators $\mathcal{L}_\mu$ and $\mathcal{D}_\mu$ obviously coincide. The operator $\mathcal{L}_\mu$ has already been analyzed in [15, Lemma 1.10], containing the proof of the following Lemma:

**Lemma 8.3.** *The operator $\mathcal{L}_\mu = \mathcal{D}_\mu$ is positive semi-definite with* $\mathrm{rk}\, \mathcal{L}_\mu \leq f^4$.

This spectral property immediately reveals the solution of the causal variational principle:

**Proposition 8.4.** *Let $\mathcal{F}$ be the set of hermitian $f \times f$-matrices of rank one with non-trivial eigenvalue $\alpha > 0$, let $\mathcal{D}$ be the function on $\mathcal{F} \times \mathcal{F}$ defined in* (8.2.6)*. Then the minimal action of the corresponding variational principle* (6.1.5) *is*

$$\mathcal{S}_{\min} = \mathcal{S}[\mu] = \frac{\alpha^4}{f(f+1)}\,, \tag{8.2.8}$$

*where $\mu$ denotes the homogenizer. Each minimizer is generically timelike.*

*Proof.* According to Lemma 8.3, we can apply Proposition 6.6, yielding that the minimal action is given by

$$\mathcal{S}_{\min} = \mathcal{S}[\mu] = \ell_\mu(x) \quad \text{for all} \quad x \in \mathcal{F}.$$

Representing elements in $\mathcal{F}$ as in (8.2.5) and using formula (8.2.7) for the homogenizer, we obtain for $x = \alpha |e_1)(e_1|$

$$\mathcal{S}_{\min} = \ell_\mu(x) = \int_{\mathcal{F}} \frac{1}{2}\,\alpha^4\,|u_1|^4\,d\mu = \frac{\alpha^4}{\mathrm{vol}(S^{2f-1})} \int_{\mathbb{C}^f} |u_1|^4\,\delta\big(\|u\|^2 - 1\big)\,du\,. \tag{8.2.9}$$

The function $g : \mathbb{C}^f \to \mathbb{R}$ defined as $g(u) = |u_1|^4 \delta\big(\|u\|^2 - 1\big)$ satisfies

$$g(Uu) = g(u) \quad \text{for all} \quad U = \left(\begin{smallmatrix} e^{i\varphi} & 0 \\ 0 & A \end{smallmatrix}\right) \in \mathrm{U}(f),\ \ \varphi \in [0, 2\pi),\ A \in \mathrm{U}(f-1).$$

Thus the integral on the right hand side of equation (8.2.9) simplifies to

$$\mathcal{S}_{\min} = \alpha^4\,\frac{\mathrm{vol}(S^{2f-3})(2\pi)}{\mathrm{vol}(S^{2f-1})} \int_0^\infty du_1 \int_0^\infty du_2\ \ u_1^5\,u_2^{2f-3}\,\delta(u_1^2 + u_2^2 - 1).$$

Using the generalized scaling property (8.1.1) applied on the $u_2$-integral and formula (8.1.2) for the area of the sphere, one calculates

$$\mathcal{S}_{\min} = \frac{\alpha^4\,\Gamma(f)}{\Gamma(f-1)} \int_0^\infty du_1\,u_1^5\,(1-u_1^2)^{f-2}\,\Theta(1-u_1^2) = \frac{\alpha^4\,\Gamma(f)}{\Gamma(f-1)} \int_0^1 du_1\,u_1^5\,(1-u_1^2)^{f-2}.$$

Substituting $u_1^2 = s$, the last expression can be transformed to

$$\mathcal{S}_{\min} = \frac{\alpha^4\,\Gamma(f)}{2\,\Gamma(f-1)} \int_0^1 ds\ s^2(1-s)^{f-2} = \frac{\alpha^4\,\Gamma(f)}{2\,\Gamma(f-1)} B(3, f-1),$$

where in the last step we used the definition of the Beta function (8.1.4). Representing the Beta function via the $\Gamma$-function, we finally obtain

$$\mathcal{S}_{\min} = \frac{\alpha^4\,\Gamma(f)}{2\,\Gamma(f-1)}\,\frac{\Gamma(3)\Gamma(f-1)}{\Gamma(f+2)} = \frac{\alpha^4}{f(f+1)}.$$

Since the functions $\mathcal{L}$ and $\mathcal{D}$ coincide, the eigenvalue $\nu_0$ of the operator $\mathcal{D}_\mu$ corresponding to the constant function $1_{\mathcal{F}}$ is given by $\nu_0 = \ell_\mu(x) = \mathcal{S}_{\min}$ . Proposition 6.15 yields that each minimizer is generically timelike. □

We remark that the value of the minimal action fits with the numerical values of Table 4.1 for $\alpha = f$. We conclude that the numerically calculated solutions define generically timelike minimizers, supported at only a finite number of points with equal weighting factors. The additional freedom of the variational principle in Section 4.3 in the choice of the non-vanishing eigenvalue did not yield a smaller action.

## 8.3 Construction of the Homogenizer

We now apply the attention to the case $\alpha, \beta > 0$. Thus $\mathcal{F}$ is the set of hermitian matrices of rank two with non-trivial simple eigenvalues $\alpha, -\beta$. As stated in Section 3.2, the space $\mathcal{F}$ can be identified with the flag manifold $\mathcal{F}_{1,2}(\mathbb{C}^f)$. We remember that the elements of the flag manifold were represented in (3.2.14) as

$$x = \alpha\, |u)(u| - \beta\, |v)(v| \quad \text{with} \quad u, v \in \mathbb{C}^f,\ \|u\| = 1 = \|v\|,\ u \perp v,$$

and that the function $\mathcal{D}$ was defined in (2.4.30) by

$$\mathcal{D} : \mathcal{F} \times \mathcal{F} \to \mathbb{R}, \quad \mathcal{D}(x, y) = \mathrm{Tr}\Big((xy)^2\Big) - \frac{1}{2}\,\mathrm{Tr}\,(xy)^2\,. \tag{8.3.10}$$

We now refer to the task constructing a homogenizer, see Definition 6.5.

**Proposition 8.5.** *Let the measure $\mu$ on $\mathcal{F}$ be defined as*

$$d\mu = \frac{4}{\mathrm{vol}(S^{2f-1})\mathrm{vol}(S^{2f-3})}\, \delta\big(\mathrm{Re}\ (u|v)\big)\, \delta\big(\mathrm{Im}\,(u|v)\,\big)\, \delta\big(\|u\|^2 - 1\big)\, \delta\big(\|v\|^2 - 1\big)\, du\, dv,$$

*where $du$ and $dv$ denotes the Lebesgue measure on $\mathbb{C}^f$. Then the measure $\mu$ defines a measure in $\mathfrak{M}$, and $\mu$ is a homogenizer of the function $\mathcal{D}$ given by* (8.3.10).

*Proof.* The measure $\mu$ is a regular Borel measure. In order to prove the normalization, we define the function $g$ on $\mathbb{C}^f$ as

$$g(u) := \int_{\mathbb{C}^f} dv\ \delta\big(\|u\|^2 - 1\big)\, \delta\big(\|v\|^2 - 1\big)\, \delta\big(\mathrm{Re}(u|v)\big)\, \delta\big(\mathrm{Im}(u|v)\big)$$

The function $g$ is $\mathrm{U}(f)$-invariant. Using the scaling property of the delta function and formula (8.1.3), for any $u \in \mathbb{C}^f$ with $r = \|u\| > 0$ one obtains

$$\begin{aligned} g(u) = g(re_1) &= \delta(r^2 - 1) \int_{\mathbb{C}^f} dv\ \delta\big(\|v\|^2 - 1\big)\, \delta\big(r\ \mathrm{Re}(e_1|v)\big)\, \delta\big(r\ \mathrm{Im}(e_1|v)\big) \\ &= \frac{1}{r^2}\ \delta(r^2 - 1) \int_{\mathbb{R}^{2f-2}} dv\ \delta\big(\|v\|^2 - 1\big) = \frac{1}{2r^2}\ \delta(r^2 - 1)\ \mathrm{vol}(S^{2f-3}). \end{aligned}$$

Finally, the generalized scaling property (8.1.1) yields

$$\int_{\mathbb{C}^f} du\ g(u) = \frac{1}{2}\mathrm{vol}(S^{2f-3}) \int_{\mathbb{C}^f} du\ \frac{1}{\|u\|^2}\ \delta(\|u\|^2 - 1) = \frac{1}{4}\mathrm{vol}(S^{2f-3})\ \mathrm{vol}(S^{2f-1}).$$

Hence $\mu$ is normalized. Obviously, $\mu$ is $\mathrm{U}(f)$-invariant. Due to the $\mathrm{U}(f)$-invariance of $\mathcal{D}$, the functions $\ell_\mu$ and $\mathsf{d}_\mu$, given by (6.2.7) and (6.2.8), are constant, concluding that $\mu$ is a homogenizer. □

## 8.4 Light-Cones on the Flag Manifold

In the next step, we examine the light-cones on the flag manifold in the case $\alpha, \beta > 0$ and $f \geq 3$. To simplify the calculations, we fix $x$ and choose an eigenvector basis of $x$, whereas $y \in \mathcal{F}$ is again represented in the form (3.2.14), thus

$$x = \alpha |e_1)(e_1| - \beta |e_2)(e_2|, \quad y = \alpha |u)(u| - \beta\, |v)(v|\,, \tag{8.4.11}$$

where $e_i$ denotes the $i$-th unit vector in $\mathbb{C}^f$ and $u, v \in \mathbb{C}^f$ satisfy $\|u\| = \|v\| = 1$, $u \perp v$. For elements given by (8.4.11), the eigenvalues of the matrix product $xy$ depend only on the upper $2 \times 2$ principal submatrix $\tilde{y} = (y_{ij})_{i,j=1}^2$ of $y$. The function $\mathcal{D}$ given by (8.3.10) simplifies to

$$\mathcal{D}(x,y) = \frac{1}{2}\big(\alpha\, y_{11} + \beta\, y_{22}\big)^2 - 2\,\alpha\,\beta\,|y_{12}|^2. \tag{8.4.12}$$

According to Lemma 3.1, the hermitian matrix $\tilde{y} \in \mathrm{Mat}(2 \times 2, \mathbb{C})$ can be represented as

$$\tilde{y} = \kappa\, \mathbb{1} + \vec{p} \cdot \vec{\sigma} \quad \text{with} \quad \kappa \in \mathbb{R},\ \vec{p} \in \mathbb{R}^3, \tag{8.4.13}$$

where the parameter $\kappa$ and the Bloch vector $\vec{p}$ are explicitly given by

$$\kappa = \tfrac{\alpha}{2}(|u_1|^2 + |u_2|^2) - \tfrac{\beta}{2}(|v_1|^2 + |v_2|^2), \quad \vec{p} = \begin{pmatrix} \mathrm{Re}(\alpha\, u_1 \overline{u}_2 - \beta\, v_1 \overline{v}_2) \\ \mathrm{Im}(\alpha\, u_1 \overline{u}_2 - \beta\, v_1 \overline{v}_2) \\ \frac{\alpha}{2}(|u_1|^2 - |u_2|^2) - \frac{\beta}{2}(|v_1|^2 - |v_2|^2) \end{pmatrix}. \tag{8.4.14}$$

In particular, the submatrix $\hat{x}$ of the fixed matrix $x$ can be written as in formula (8.4.13) with $\kappa = \frac{\alpha - \beta}{2}$ and $\vec{p} = \frac{\alpha+\beta}{2}\vec{e}_3$, where $\vec{e}_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ denotes the north pole on the sphere $S^2$.

Now let $y \in \mathcal{F}$ be an arbitrary element with principal submatrix given by (8.4.13). Denoting with $p = \|\vec{p}\|$ the length of the Bloch vector, we define $\vec{w} \in S^2$ via $\vec{p} = p\vec{w}$. The eigenvalues of the submatrix $\tilde{y}$ are given by $\kappa \pm p$, which are according to the inclusion principle (see [19, Theorem 4.3.15]) bounded by the eigenvalues of $y$ as

$$-\beta \leq \kappa - p \leq 0 \leq p + \kappa \leq \alpha. \tag{8.4.15}$$

According to formula (3.1.9), the function $\mathcal{D}$ can be written as

$$\mathcal{D}(x,y) = \frac{1}{2}\Big((\alpha+\beta)\kappa + p\,(\alpha-\beta)\,(\vec{e}_3 \cdot \vec{w})\Big)^2 - 2\,\alpha\,\beta\,p^2\,\Big(1 - (\vec{e}_3 \cdot \vec{w})^2\Big). \tag{8.4.16}$$

This function depends on the angle $\vartheta \in [0, \pi]$ given by $\cos\vartheta = \vec{e}_3 \cdot \vec{w}$ between the north pole $\vec{e}_3$ and the vector $\vec{w}$, but now also on the parameters $\kappa$ and $p$. Keeping these parameters fixed, we discuss the behavior of the function $\mathcal{D}$ depending on $\vartheta$ distinguishing the following cases:

$p = 0$: Formula (8.4.15) yields $\kappa = 0$, thus $\mathcal{D}(\vartheta) = 0$ for all $\vartheta \in [0, \pi]$.

$p = \kappa$: The function $\mathcal{D}$ is non-negative with a double zero at $\cos\vartheta = \frac{\alpha-\beta}{\alpha+\beta}$.

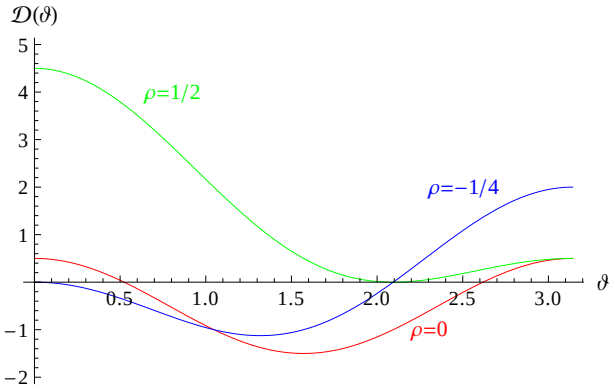



Figure 8.1: The function $\mathcal{D}(\vartheta)$ for $\tau = 2$ and $p = \frac{1}{2}$.

$p > 0$, $p \neq \kappa$: The function $\mathcal{D}(\vartheta)$ has two distinct zeros in $[0, \pi]$ given by

$$\cos\vartheta_\pm = \frac{\kappa\,(\alpha-\beta) \pm \sqrt{\alpha\,\beta\,(p^2-\kappa^2)}}{p\,(\alpha+\beta)}, \tag{8.4.17}$$

and is negative between the two zeros.

For fixed $\kappa, p$, the subset $\{\vec{w} \in S^2 \;:\; \mathcal{D}(\vec{w}) > 0\}$ of $S^2$ describes a spherical segment. These subsets differ for $f \geq 3$ from the light-cones on the sphere in the case $f = 2$, discussed in Section 5.1. The maximal value of the function $\mathcal{D}$ is either obtained for $\vec{e}_3 \cdot \vec{w} = 1$ or $\vec{e}_3 \cdot \vec{w} = -1$, and is positive in all cases. For an illustration, we use the parametrization (5.1.9), where the function $\mathcal{D}$ may be rewritten as

$$\mathcal{D}(\vartheta) = 2\Big((p\cos\vartheta \;+\kappa\,\tau)^2 - p^2(\tau^2-1)\sin^2\vartheta\Big). \tag{8.4.18}$$

Exemplary plots of the function $\mathcal{D}(\vartheta)$ for fixed $\tau$ and $p$, and fixed but different values of $\rho$ are shown in Figure 8.1.

Concluding, we state the light-cones of Definition 6.3 in the general case of prescribed eigenvalues $\alpha$ and $-\beta$ using the zeros (8.4.17) of the function $\mathcal{D}$:

$$\begin{aligned}
\mathcal{I}(x) =& \Big\{ y \in \mathcal{F} \text{ with } \tilde{y} = \kappa\,\mathbb{1}_2 + p\,\vec{w}\cdot\vec{\sigma} \;:\; \kappa,\, p \in \mathbb{R} \text{ satisfy } \;(8.4.15),\; p > 0, \\
& \quad \vec{w} \in S^2 \text{ with } \vec{w}\cdot\vec{e}_3 \in [-1, \cos\vartheta_-) \cup (\cos\vartheta_+, 1] \Big\}, \\
\mathcal{J}(x) =& \Big\{ y \in \mathcal{F} \;\text{ with }\; \tilde{y} = \kappa\,\mathbb{1}_2 + p\,\vec{w}\cdot\vec{\sigma} \;:\; \kappa,\, p \in \mathbb{R} \text{ satisfy } \;(8.4.15),\; p > 0, \\
& \quad \vec{w} \in S^2 \text{ with } \vec{w}\cdot\vec{e}_3 \in [-1, \cos\vartheta_-] \cup [\cos\vartheta_+, 1] \Big\} \cup \Big\{ y \in \mathcal{F} \;\text{ with }\; \tilde{y} = 0 \Big\}, \\
\mathcal{K}(x) =& \Big\{ y \in \mathcal{F} \;\text{ with }\; \tilde{y} = \kappa\,\mathbb{1}_2 + p\,\vec{w}\cdot\vec{\sigma} \;:\; \kappa,\, p \in \mathbb{R} \text{ satisfy } \;(8.4.15),\; p > 0, \\
& \quad \vec{w} \in S^2 \text{ with } \vec{w}\cdot\vec{e}_3 = \cos\vartheta_- \text{ or } \vec{w}\cdot\vec{e}_3 = \cos\vartheta_+ \} \Big\} \cup \Big\{ y \in \mathcal{F} \;\text{ with }\; \tilde{y} = 0 \Big\}.
\end{aligned} \tag{8.4.19}$$

## 8.5 Calculation of the Measures of the Light-Cones

We now calculate the measure of the open light-cone $\mathcal{I}(x)$ with respect to the homogenizer $\mu$ defined in Proposition 8.5. For this purpose, we first calculate the measure of the family of matrices, whose upper $2 \times 2$ principal submatrices coincide with a given $2 \times 2$ matrix $\kappa_0 + \vec{p}_0 \cdot \vec{\sigma}$, where $\vec{p}_0 \in \mathbb{R}^3$ and $\kappa_0 \in \mathbb{R}$ satisfy (8.4.15). The measure of these matrices, denoted as $\mu(\kappa_0, \vec{p}_0)$, is calculated as

$$\mu(\kappa_0, \vec{p}_0) = \int_{\mathcal{F}} d\mu \; \delta\big(\kappa(u,v) - \kappa_0\big) \; \delta^3\big(\vec{p}(u,v) - \vec{p}_0\big). \tag{8.5.20}$$

Here we denote $\kappa(u,v)$ and $\vec{p}(u,v)$ as the parameter and Bloch vector according via (8.4.14) to an element $y \in \mathcal{F}$ with normalized eigenvectors $u, v \in \mathbb{C}^f$ and submatrix $\tilde{y}$ . The value $\mu(\kappa_0, \vec{p}_0)$ only depends on the length of the vector $\vec{p}_0$:

**Lemma 8.6.** *The function $\mu(\kappa_0, \vec{p}_0)$ is $\mathrm{SO}(3)$-invariant in its second argument,*

$$\mu(\kappa_0, \vec{p}_0) = \mu(\kappa, R\,\vec{p}_0) \quad \textit{for all} \quad R \in \mathrm{SO}(3).$$

*Proof.* Let $R \in \mathrm{SO}(3)$. According to (3.1.6), there exists $V \in SU(2)$ such that

$$\kappa\, \mathbb{1}_2 + (R\,\vec{p}) \cdot \vec{\sigma} = \kappa\, \mathbb{1}_2 + V\, (\vec{p} \cdot \vec{\sigma})\, V^{-1} \;\text{ for all }\; \kappa \in \mathbb{R},\; \vec{p}_0 \in \mathbb{R}^3.$$

Using the $\mathrm{U}(f)$-invariance of the measure and the generalized scaling property in higher dimensions, one calculates for $U = \left(\begin{smallmatrix} V & 0 \\ 0 & \mathbb{1}_{f-2} \end{smallmatrix}\right) \in \mathrm{U}(f)$

$$\begin{aligned}
\mu(\kappa_0, R^\dagger \vec{p}_0) &= \int_{\mathcal{F}} d\mu \; \delta\big(\kappa(u,v) - \kappa_0\big) \; \delta^3\big(\vec{p}(u,v) - R^\dagger \vec{p}_0\big) \\
&= \int_{\mathcal{F}} d\mu \; \delta\big(\kappa(u,v) - \kappa_0\big) \; \delta^3\big(R\,\vec{p}(u,v) - \vec{p}_0\big) \\
&= \int_{\mathcal{F}} d\mu \; \delta\big(\kappa(Vu,Vv) - \kappa_0\big) \; \delta^3\big(\vec{p}(Vu,Vv) - \vec{p}_0\big) \\
&= \int_{\mathcal{F}} d\mu \; \delta\big(\kappa(u,v) - \kappa_0\big) \; \delta^3\big(\vec{p}(u,v) - \vec{p}_0\big) = \mu(\kappa_0, \vec{p}_0).
\end{aligned}$$

□

We will use this Lemma to calculate the measure of matrices with prescribed principal submatrix:

**Proposition 8.7.** *Let $\vec{p}_0 \in \mathbb{R}^3 \backslash \{0\}$ and $\kappa_0 \in \mathbb{R}$ be elements satisfying (8.4.15). The measure $\mu(\kappa_0, \vec{p}_0)$ of elements $y$ in $\mathcal{F}$ whose principal upper submatrix $\tilde{y}$ is prescribed as $\kappa_0 \mathbb{1}_2 + \vec{p}_0 \cdot \vec{\sigma}$ is given by*

$$\mu(\kappa_0, \vec{p}_0) = \frac{(f-1)(f-2)^2}{p_0\, \pi\, (\alpha+\beta)\, (\alpha\beta)^{f-2}} \Big((\alpha - p_0 - \kappa_0)(\beta - p_0 + \kappa_0)\Big)^{f-3}. \tag{8.5.21}$$

*Proof.* According to Lemma 8.6, we can assume that $\vec{p}_0 = p_0 \vec{e}_3$ with $p_0 = \|\vec{p}_0\| > 0$. After substituting $u_i \to \sqrt{\alpha}\, u_i$ and $v_i \to \sqrt{\beta}\, v_i$, the measure $\mu(\rho_0, \vec{p}_0)$ given by (8.5.20) is calculated as

$$\begin{aligned}\mu(\kappa_0, p_0) &= \frac{4}{\mathrm{vol}(S^{2f-1})\mathrm{vol}(S^{2f-3})} \frac{4}{(\alpha\beta)^{f-2}} \int_{\mathbb{C}^f} du \int_{\mathbb{C}^f} dv\; \delta\Big(\|u\|^2 - \alpha\Big)\, \delta\Big(\|v\|^2 - \beta\Big) \\ &\quad \delta\Big(\mathrm{Re}(u|v)\Big)\, \delta\Big(\mathrm{Im}(u|v)\Big) \delta\Big((|u_1|^2 + |u_2|^2) - (|v_1|^2 + |v_2|^2) - 2\kappa_0\Big) \\ &\quad \delta\Big(\mathrm{Re}(u_1 \overline{u}_2 - v_1 \overline{v}_2)\Big) \delta\Big(\mathrm{Im}(u_1 \overline{u}_2 - v_1 \overline{v}_2)\Big)\, \delta\Big(|u_1|^2 - |u_2|^2 - (|v_1|^2 - |v_2|^2) - 2p_0\Big) \\ &=: c \int_{C^f} du \int_{\mathbb{C}^f} dv\; g(u, v).\end{aligned}$$

We first assume that $f \geq 4$ and simplify the expression as follows:

1) Since it is $\int_{\mathbb{C}^f} dv\; g(u,v) = \int_{\mathbb{C}^f} dv\; g(Uu, v)$ for $U = \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & A \end{pmatrix} \in U(f)$ where $A \in \mathrm{U}(f-2)$, the $u$-integral simplifies to

$$\mu(\kappa_0, p_0) = c\, \mathrm{vol}(S^{2f-5}) \int_{\mathbb{C}} du_1 \int_{\mathbb{C}} du_2 \int_0^\infty du_3\; u_3^{2f-5} \int_{\mathbb{C}^f} dv\; g(u_1, u_2, u_3, v),$$

2) Since it is $\int du\; g(u,v) = \int du\; g(u, Uv)$ for $U = \begin{pmatrix} \mathbb{1}_3 & 0 \\ 0 & A \end{pmatrix} \in U(f)$ with $A \in \mathrm{U}(f-3)$, the $v$-integral simplifies to

$$\mu(\kappa_0, p_0) = \ldots\, \mathrm{vol}(S^{2f-7}) \int_{\mathbb{C}^3} dv \int_0^\infty dv_4\; v_4^{2f-7}\; g(u_1, u_2, u_3, v_1, \ldots, v_4).$$

3) Since it is $\int_{\mathbb{C}} du_2 \int_{\mathbb{C}} dv_1 \int_{\mathbb{C}} dv_2\; g(e^{i\varphi} u_1, \ldots) = \int_{\mathbb{C}} du_2 \int_{\mathbb{C}} dv_1 \int_{\mathbb{C}} dv_2\; g(u_1, \ldots)$ for $\varphi \in [0, 2\pi)$, the $u_1$-integral simplifies to

$$\mu(\kappa_0, p_0) = \ldots\, (2\pi) \int_0^\infty u_1\; du_1 \ldots.$$

4) Using the generalized scaling property, the transformation $(u_2, v_2) \mapsto e^{i\varphi}(u_2, v_2)$ with $\varphi \in [0, 2\pi)$ does not change the integrand and thus simplifies the $u_2$-integral to

$$\mu(\kappa_0, p_0) = \ldots\, (2\pi) \int_0^\infty u_2\; du_2 \ldots.$$

5) The transformation $(v_1, v_2, v_3) \mapsto e^{i\varphi}(v_1, v_2, v_3)$ with $\varphi \in [0, 2\pi)$ similarly simplifies the $v_1$-integral to

$$\mu(\kappa_0, p_0) = \ldots\, (2\pi) \int_0^\infty v_1\; dv_1 \ldots.$$

Combining all this, one obtains

$$\begin{aligned}\mu(\kappa_0, p_0) =& c \int_0^\infty du_1 \int_0^\infty du_2 \int_0^\infty du_3 \int_0^\infty dv_1 \int_{\mathbb{C}} dv_2 \int_{\mathbb{C}} dv_3 \int_0^\infty dv_4 \\ & \times u_1\, u_2\, u_3^{2f-5}\, v_1\, v_4^{2f-7} \delta\Big(\|u\|^2 - \alpha\Big) \delta\Big(\|v\|^2 - \beta\Big) \\ & \times \delta\Big(\mathrm{Re}(u|v)\Big)\; \delta\Big(u_2 \mathrm{Im} v_2 + u_3 \mathrm{Im} v_3\Big)\; \delta\Big(u_1 u_2 - v_1 \mathrm{Re} v_2\Big) \delta\Big(v_1 \mathrm{Im} \overline{v}_2\Big) \\ & \times \delta\Big(u_1^2 + u_2^2 - v_1^2 - |v_2|^2 - 2\kappa_0\Big)\; \delta\Big(u_1^2 - u_2 - v_1^2 + |v_2|^2 - 2p_0\Big)\end{aligned}$$

with the new constant

$$\begin{aligned} c &= \frac{4}{\mathrm{vol}(S^{2f-1})\mathrm{vol}(S^{2f-3})} \frac{4}{(\alpha\beta)^{f-2}} \mathrm{vol}(S^{2f-5})\mathrm{vol}(S^{2f-7})(2\pi)^3 \\ &= \frac{4}{(\alpha\beta)^{f-2}} \frac{2^5}{\pi} (f-1)(f-2)^2(f-3), \end{aligned}$$

where we used formula (8.1.2) for the volume of a $n$-sphere.

We now integrate the $\delta$-functions using the generalized scaling property (8.1.1) and thus execute the real integrals step by step. To shorten the notation, we use a curly brace, where in the first line the exchange rule for the variable and in the second line the additional factor the function has to be multiplied with is stated.

i) Using $\delta(v_1 \,\mathrm{Im}\, \overline{v}_2)$, the integral over $\mathrm{Im}\, v_2$ yields

$$\left\{ \begin{matrix} \mathrm{Im}\, v_2 = 0 \\ \times \frac{1}{v_1} \end{matrix} \right\}$$

ii) The term $\delta(\mathrm{Im}\,(u|v))$ simplifies to $\delta(u_3 \,\mathrm{Im}\, v_3)$, thus the integral over $\mathrm{Im}\, v_3$ yields

$$\left\{ \begin{matrix} \mathrm{Im}\, v_3 = 0 \\ \times \frac{1}{u_3} \end{matrix} \right\}$$

After this, the complex numbers $v_2, v_3$ are real, and we write $v_i$ instead of $\mathrm{Re} v_i$.

iii) The term $\delta(\mathrm{Re}(u|v))$ simplifies to $\delta(u_1 v_1 + u_2 v_2 + u_3 v_3)$, carrying out the $v_3$-integral yields

$$\left\{ \begin{matrix} v_3 = -\frac{u_1 v_1 + u_2 v_2}{u_3} \\ \times \frac{1}{u_3} \end{matrix} \right\}$$

iv) The integral over $v_2$ yields using $\delta(\, u_1 u_2 - v_1 v_2)$

$$\left\{ \begin{matrix} v_2 = \frac{u_1 u_2}{v_1} \\ \times \frac{1}{v_1} \end{matrix} \right\}$$

v) The integral over $u_1$ yields using $\delta(u_1^2+u_2^2-v_1^2-\frac{u_1^2u_2^2}{v_1^2}-2\kappa_0)$

$$\left\{\begin{array}{c} u_1 = v_1\sqrt{\frac{v_1^2-u_2^2+2\kappa_0}{v_1^2-u_2^2}} \\ \times\left(2u_1(1-\frac{u_2^1}{v_1^2})\right)^{-1}\Theta\left(v_1^2\frac{v_1^2-u_2^2+2\kappa_0}{v_1^2-u_2^2}\right)\end{array}\right\}$$

vi) Now $\delta(2p-2p_0)$ is given as $\delta(2\frac{u_2^2+v_1^2}{v_1^2-u_2^2}\kappa_0-2p_0)$, thus the integral over $u_2$ yields

$$\left\{\begin{array}{c} u_2 = v_1\sqrt{\frac{p_0-\kappa_0}{p_0+\kappa_0}} \\ \times\frac{(u_2^2-v_1^2)^2}{8u_2v_1^2\kappa_0}\Theta\left(v_1^2\frac{p_0-\kappa_0}{p_0+\kappa_0}\right)\end{array}\right\}$$

vii) The integral over $u_3$ yields using $\delta(\|u\|^2-\alpha)$

$$\left\{\begin{array}{c} u_3 = \sqrt{\alpha-u_1^2-u_2^2} \\ \times\frac{1}{2u_3}\Theta(\alpha-u_1^2-u_2^2)\end{array}\right\}$$

viii) The integral over $v_4$ yields using $\delta(\|v\|^2-\beta)$

$$\left\{\begin{array}{c} v_4 = \sqrt{\beta-v_1^2-v_2^2-v_3^2} \\ \times\frac{1}{2v_4}\Theta(\beta-v_1^2-v_2^2-v_3^2)\end{array}\right\}$$

Having executed all delta functions, a one-dimensional integral remains

$$\mu(\kappa_0,p_0) = c\int_0^\infty dv_1\,\frac{v_1}{32(p_0+\kappa_0)}\,(u_3v_4)^{2f-8}\,\Theta(u_1^2)\Theta(u_2^2)\Theta(u_3^2)\Theta(v_4^2),$$

where the variables $u_1,u_2,u_3,v_2,v_3,v_4$ depend on $v_1$, and $c$ is a new constant. The first two Heaviside functions yield the inequality constraints

$$u_1^2 = \frac{p_0+\kappa_0+v_1^2}{v_1^2} \geq 0,$$
$$u_2^2 = \frac{p_0-\kappa_0}{p_0+\kappa_0} \geq 0,$$

which are satisfied according to the required relation (8.4.15). The argument of $\Theta(u_3^2)$ can be transformed to

$$u_3^2 = \frac{1}{p_0+\kappa_0}\Big((\alpha-p_0-\kappa_0)(p_0+\kappa_0)-2p_0v_1^2\Big),$$

describing a downward opened parabola with positive zero

$$b_1 = \frac{1}{\sqrt{2p_0}}\sqrt{(\alpha-p_0-\kappa_0)(p_0+\kappa_0)}.$$

The Heaviside function $\Theta(v_4^2)$ yields the inequality

$$(\alpha-p_0-\kappa_0)(\beta-p_0+\kappa_0)(p_0+\kappa_0)-2p_0(\alpha+\beta)v_1^2 \geq 0,$$

and thus again a downward opened parabola with positive zero

$$b_2 = \frac{1}{\sqrt{2p_0(\alpha+\beta)}} \sqrt{(\alpha - p_0 - \kappa_0)(\beta - p_0 + \kappa_0)(p_0 + \kappa_0)}.$$

According to (8.4.15), the square roots are well-defined, and it is $b_2 \leq b_1$. Consequently, it remains to calculate

$$\mu(\kappa_0, p_0) = \frac{c}{32(p_0+\kappa_0)} \int_0^{b_2} v_1 \left( (\alpha - p_0 - \kappa_0)(\beta - p_0 + \kappa_0) - \frac{2p_0(\alpha+\beta)}{p_0+\kappa_0} v_1^2 \right)^{f-4} dv_1.$$

Carrying out the integral, yields formula (8.5.21).
In the case $f = 3$, a similar calculation yields the formula for $f = 3$. □

We now discuss formula (8.5.21): For a check, we integrate over $p$ and $\kappa$ satisfying (8.4.15). As the function $\mu(\kappa, \vec{p})$ is SO(3)-symmetric in its second argument, we have to calculate

$$4\pi \int_{-\infty}^{\infty} d\kappa \int_0^{\infty} dp\, p^2\, \mu(\kappa, p)\, \Theta(p-\kappa)\, \Theta(p+\kappa)\, \Theta(\beta+p-\kappa)\, \Theta(\alpha-p-\kappa).$$

Substituting $p + \kappa = \alpha\, s$ and $p - \kappa = \beta\, t$, the integral transforms to

$$\begin{aligned} &\alpha\beta \int_0^1 ds \int_0^1 dt\, (\alpha\, s + \beta\, t)\, \frac{(f-1)(f-2)^2}{(\alpha+\beta)\big(\alpha\beta\big)^{f-2}} \Big( (\alpha - \alpha\, s)(\beta - \beta\, t) \Big)^{f-3} \\ &= (f-1)\, (f-2)^2\, B(2, f-2)\, B(1, f-2) = 1. \end{aligned}$$

As requested, the integral over all principal submatrices yields the total volume of the flag manifold $\mu(\mathcal{F}) = 1$.

Using formula (8.5.21), we can calculate the measure of the light-cone:

**Theorem 8.8.** *Let $x \in \mathcal{F}$. The measure of the open light-cone of $x$ is*

$$\mu\big(\mathcal{I}(x)\big) = 1 - \frac{(f-1)\, \alpha\beta\, \pi\, \Gamma(f-1)^2}{(\alpha+\beta)^2\, \Gamma\left(f - \frac{1}{2}\right)^2}\,. \tag{8.5.22}$$

*Proof.* Since the measure is $\mathrm{U}(f)$-invariant, we can choose $x, y \in \mathcal{F}$ as in (8.4.11), where the principal submatrix of $y$ is given by (8.4.13) with $\vec{p} = p\, \vec{w}$, $\vec{w} \in S^2$. According to formula (8.4.19) for the open light-cone, the measure of it is given by

$$\begin{aligned} \mu\big(\mathcal{I}(x)\big) &= \int_{-\infty}^{\infty} d\kappa \int_0^{\infty} dp \int_{S^2} d\vec{w}\, p^2\, \mu(\kappa, p)\, \Theta(p-\kappa)\, \Theta(p+\kappa) \\ &\qquad \times \Theta(\beta+p-\kappa)\, \Theta(\alpha-p-\kappa)\, \Theta(\mathcal{D}(x,y)) \\ &= (2\pi) \int_{-\infty}^{\infty} d\kappa \int_0^{\infty} dp\, p^2 \int_0^{\pi} d\vartheta\, \mu(\kappa, p)\, \Theta(p-\kappa)\, \Theta(p+\kappa) \\ &\qquad \times \Theta(\beta+p-\kappa)\, \Theta(\alpha-p-\kappa)\, \Theta(\mathcal{D}(\vartheta))\, \sin\vartheta. \end{aligned}$$

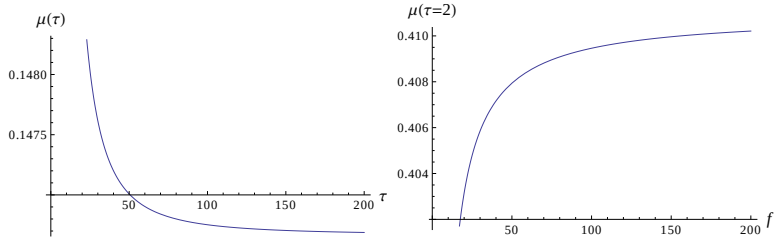



Figure 8.2: The function $\mu$ for $f = 4$ varying $\tau$ (left) and the behavior of $\mu$ for $\tau = 2$ fixed varying $f$ (right).

Using formula (8.4.17) for the zeros of the function $\mathcal{D}$, the part depending on $\vartheta$ can be calculated as

$$\int_0^\pi d\vartheta\ \sin\vartheta\ \Theta(\mathcal{D}(\vartheta)) = \left(\int_0^{\vartheta_+} + \int_{\vartheta_-}^\pi\right) d\vartheta\ \sin\vartheta = 2 - \frac{4\sqrt{\alpha\beta(p^2-\kappa^2)}}{p(\alpha+\beta)}.$$

Substituting $p+\kappa = \alpha\ s$ and $p-\kappa = \beta\ t$, we obtain using formula (8.5.21)

$$\begin{aligned}\mu\big(\mathcal{I}(x)\big) &= \tfrac{(f-1)(f-2)^2}{(\alpha+\beta)} \int_0^1 ds \int_0^1 dt\ (\alpha\ s+\beta\ t)\left(1-\tfrac{4\,\alpha\,\beta\,\sqrt{s\,t}}{(\alpha\ s+\beta\ t)(\alpha+\beta)}\right)\Big((1-s)(1-t)\Big)^{f-3} \\ &= 1 - \tfrac{4(f-1)(f-2)^2\alpha\beta}{(\alpha+\beta)^2}\ B\left(\tfrac{3}{2}, f-2\right)^2 = 1 - \tfrac{4(f-1)(f-2)^2\alpha\beta}{(\alpha+\beta)^2}\left(\frac{\Gamma(\frac{3}{2})\Gamma(f-2)}{\Gamma(f-\frac{1}{2})}\right)^2.\end{aligned}$$

A reformulation of the $\Gamma$-functions yields the claimed formula. □

Discussing formula (8.5.22) of the measure of the light-cone, we again prescribe the eigenvalues as $1 \pm \tau$ for $\tau > 1$, see (5.1.9), and obtain

$$\mu\big(\mathcal{I}(x)\big) = 1 - \frac{(f-1)\ (\tau^2-1)\ \pi\ \Gamma(f-1)^2}{4\ \tau^2\ \Gamma\left(f-\frac{1}{2}\right)^2}. \tag{8.5.23}$$

If $f = 2$, we obtain

$$\mu\big(\mathcal{I}(x)\big) = \frac{1}{\tau^2}.$$

This is just the volume of a spherical cap of opening angle $2\vartheta_{\max}$, and fits with the statements of Chapter 5. In particular, $\mu\big(\mathcal{I}(x)\big) \to 0$ for $\tau \to \infty$.

In the case $f = 3$, we obtain

$$\mu\big(\mathcal{I}(x)\big) = \frac{1}{9} + \frac{8}{9\tau^2}.$$

The measure is monotonically decreasing and converges to a positive constant if $\tau \to \infty$. The measure of the light-cone behaves similar in the case $f = 4$, where we calculate

$$\mu\big(\mathcal{I}(x)\big) = \frac{11}{75} + \frac{64}{75\tau^2}.$$

The behavior of the measure is exemplarily shown in Figure 8.2 and can be stated as follows:

**Lemma 8.9.** *Let $\mu(\mathcal{I}(x))$ denote the measure of the light-cone, given by* (8.5.23) .

*i) Increasing $\tau$ and keeping $f$ fixed, the measure of the light-cone is monotonically decreasing.*

*ii) Increasing $f$ and keeping $\tau$ fixed, the measure of the light-cone is monotonically increasing.*

*iii) The measure behaves asymptotically as*

$$\begin{aligned}
&\mu\big(\mathcal{I}(x)\big) \longrightarrow 1 + \frac{\pi}{4}\left(\frac{1}{\tau^2} - 1\right) \quad \text{for} \quad f \to \infty, \\
&\mu\big(\mathcal{I}(x)\big) \longrightarrow 1 - \frac{(f-1)\ \pi\, \Gamma(f-1)^2}{4\ \Gamma\left(f-\frac{1}{2}\right)^2} \quad \text{for} \quad \tau \to \infty, \\
&\mu\big(\mathcal{I}(x)\big) \longrightarrow 1 - \frac{\pi}{4} \quad \text{for} \quad f, \tau \to \infty.
\end{aligned}$$

*Proof.* The first statement is obvious from equation (8.5.22). In order to prove the second statement, we denote the measure of the light-cone of $f$ particles as $\mu_f(I(x))$. Using the basic property of the $\Gamma$-function $\Gamma(z+1) = z\Gamma(z)$, it is

$$\begin{aligned}
\mu_{f+1}(\mathcal{I}(x)) - \mu_f(\mathcal{I}(x)) &= \frac{\pi(\tau^2-1)}{4\tau^2}\left(\frac{(f-1)\Gamma(f-1)^2}{\Gamma\left(f-\frac{1}{2}\right)^2} - \frac{f(f-1)^2\Gamma(f-1)^2}{(f-\frac{1}{2})^2\Gamma\left(f-\frac{1}{2}\right)^2}\right) \\
&= \frac{\pi(\tau^2-1)(f-1)\Gamma(f-1)^2}{16\ \tau^2\ \left(f-\frac{1}{2}\right)^2\ \Gamma\left(f-\frac{1}{2}\right)^2} > 0.
\end{aligned}$$

The limit $\tau \to \infty$ is obvious from formula (8.5.23). Using the Sterling formula for the $\Gamma$-function $\Gamma(z) = \sqrt{\frac{2\pi}{z}}\ \left(\frac{z}{e}\right)^z \left(1 + \mathcal{O}\left(\frac{1}{z}\right)\right)$ for $z > 0, z \to \infty$, one obtains

$$\lim_{f\to\infty} \frac{f\ \Gamma(f)^2}{\Gamma\left(f+\frac{1}{2}\right)^2} = \lim_{f\to\infty} \frac{f\ (2\pi) f^{2f}\ \left(f+\frac{1}{2}\right)\ e^{2f+1}}{f\ e^{2f}\ 2\pi\ \left(f+\frac{1}{2}\right)^{2f+1}} = e\ \lim_{f\to\infty}\ \left(\frac{f}{f+\frac{1}{2}}\right)^{2f} = 1.$$

Inserting in (8.5.23), we obtain

$$\lim_{f\to\infty}\ \mu\big(\mathcal{I}(x)\big) = 1 - \frac{\pi(\tau^2-1)}{4\tau^2},$$

which completes the proof. □

In the case $f = 2$, the light-cones shrink with increasing $\tau$ to a set of measure zero. If the number of particles is increased, the light-cones shrink with increasing $\tau$ to a set of non-zero measure. This seems reasonable since the light-cone of $x$ is just determined by the upper $2 \times 2$-principal submatrix of elements in $\mathcal{F}$. If the number of particles increases, the matrices get higher dimensional. Thus there is more space to satisfy both the eigenvalue constraint and the constraint that $y$ is in the light-cone of $x$.

## 8.6 The Action of the Homogenizer

We now calculate the action of the normalized volume measure using the above results. We recall that the action of a measure $\rho \in \mathfrak{M}$ is defined as

$$\mathcal{S}[\rho] = \iint_{\mathcal{F}\times\mathcal{F}} \mathcal{L}(x,y)\, d\rho(x) d\rho(y),$$

where $\mathcal{L}$ is the positive part of the function $\mathcal{D}$ given by (8.3.10).

**Proposition 8.10.** *Let $\mu$ denote the homogenizer defined in Proposition 8.5. Then the action of $\mu$ is*

$$\mathcal{S}[\mu] = \frac{3\alpha^2\beta^2}{f-f^2} + \frac{3\pi\alpha^3\beta^3(f-1)\Gamma(f-1)^2}{(\alpha+\beta)^2\Gamma\left(f+\frac{1}{2}\right)^2} + \frac{\left(\alpha^2-\alpha\beta+\beta^2\right)^2}{f(f+1)} \tag{8.6.24}$$

*Proof.* Due to the $\mathrm{U}(f)$-invariance, it is $\mathcal{S}[\mu] = \ell_\mu(x)$ for any $x \in \mathcal{F}$. Choosing $x, y \in \mathcal{F}$ as in (8.4.11), the function $\mathcal{L}(x,y)$ just depends on $\tilde{y}$ and we obtain

$$\begin{aligned}\mathcal{S}[\mu] =& (2\pi)\int_{-\infty}^{\infty} d\kappa \int_0^\infty dp\, p^2\, \mu(\kappa,p)\Theta(p-\kappa)\Theta(p+\kappa) \\ &\times \Theta(\beta+p-\kappa)\Theta(\alpha-p-\kappa)\int_0^\pi d\vartheta\, \sin\vartheta\, \mathcal{L}(\vartheta).\end{aligned}$$

Using formula (8.4.17) for the zeros of the function $\mathcal{D}$, we calculate

$$\begin{aligned}&\int_0^\pi d\vartheta\, \sin\vartheta\, \mathcal{L}(\vartheta) = \left(\int_0^{\vartheta_+} + \int_{\vartheta_-}^\pi\right)\sin\vartheta\, \mathcal{L}(\vartheta) \\ &= \kappa^2(\alpha+\beta)^2 + \frac{1}{3}\, p^2\left(\alpha^2 - 10\alpha\beta + \beta^2\right) + \frac{16\left(\alpha\,\beta\,(p-\kappa)\,(p+\kappa)\right)^{3/2}}{3\,p\,(\alpha+\beta)}.\end{aligned}$$

Inserting and substituting $p+\kappa = \alpha\, s$ and $p-\kappa = \beta\, t$, we obtain

$$\begin{aligned}\mathcal{S}[\mu] &= \frac{(f-1)(f-2)^2}{6(\alpha+\beta)}\int_0^1 ds \int_0^1 dt\, \Big((1-s)(1-t)\Big)^{f-3} \\ &\quad\times\Big[32\left(\alpha^2\,\beta^2\,s\,t\right)^{3/2} - 9\,\alpha^2\,\beta^2\,s\,t\,(\alpha+\beta)\,(\alpha s+\beta t) + \left(\alpha^3 s^3+\beta^3 t^3\right)\left(\alpha^3+\beta^3\right)\Big] \\ &= \frac{(f-1)(f-2)^2}{6(\alpha+\beta)}\Big[32\,\alpha^3\,\beta^3\,B\left(\tfrac{5}{2}, f-2\right)^2 - 9\,\alpha^2\,\beta^2\,(\alpha+\beta)^2 \\ &\quad\times B(3,f-2)B(2,f-2) + (\alpha^3+\beta^3)^2 B(4,f-2)B(1,f-2)\Big].\end{aligned}$$

A reformulation with the $\Gamma$-functions yields formula (8.6.24). □

We can use the action of the homogenizer to estimate the minimal action as

$$\mathcal{S}[\mu] \geq \mathcal{S}_{\min}.$$

Using the parametrization (5.1.9) for $\tau > 1$, the action of the homogenizer is

$$\mathcal{S}[\mu] = \frac{2\left((f+2)\tau^4 - 6f\tau^2 - 3f + 6\right)}{f - f^3} + \frac{3\pi(f-1)\left(\tau^2-1\right)^3 \Gamma(f-1)^2}{4\tau^2 \Gamma\left(f+\frac{1}{2}\right)^2}. \quad (8.6.25)$$

In the case $f = 2$, we obtain $\mathcal{S}[\mu] = 4 - \frac{4}{3\tau^2}$, as calculated in Section 7.2.2. Regarding formula (8.6.25), we conclude that for fixed $f \geq 3$ it is $\mathcal{S}[\mu] \to \infty$ for $\tau \to \infty$. The estimate with the action of the homogenizer may thus only be useful for $\tau$ close to one.

## 8.7 Spectral Properties of Integral Operators

In order to decide whether the results of Section 6.4 can be applied, we next examine the integral operator $\mathcal{D}_\mu$ on the flag manifold.

**Lemma 8.11.** *The operator $\mathcal{D}_\mu$ has rank at most $3f^4$.*

*Proof.* We extend the method used in the proof of [15, Lemma 1.10]. Here it is more convenient to represent the element $x \in \mathcal{F}$ as

$$x = |u(x))(u(x)| - |v(x))(v(x)|\,,$$

where $u(x)$ and $v(x)$ are the eigenvectors of $x$, normalized such that

$$(u(x)|u(x)) = \alpha \qquad \text{and} \qquad (v(x)|v(x)) = \beta\,.$$

A short calculation shows that the non-trivial eigenvalues of the matrix product $xy$ coincide with the eigenvalues of the $2 \times 2$-matrix product

$$A_{xy} := \begin{pmatrix} (u(x)|u(y)) & -(u(x)|v(y)) \\ (v(x)|u(y)) & -(v(x)|v(y)) \end{pmatrix} \begin{pmatrix} (u(y)|u(x)) & -(u(y)|v(x)) \\ (v(y)|u(x)) & -(v(y)|v(x)) \end{pmatrix}.$$

Using (2.4.30), we can thus write the function $\mathcal{D}$ as

$$\mathcal{D}(x,y) = \mathrm{Tr}\left[\left(A_{xy} - \frac{1}{2}\,\mathrm{Tr}(A_{xy})\right)^2\right].$$

This makes it possible to recover $\mathcal{D}(x,y)$ as the "expectation value"

$$\mathcal{D}(x,y) = \left( \left( \begin{smallmatrix} u\otimes u^*\otimes u\otimes u^* \\ u\otimes u^*\otimes v\otimes v^* \\ v\otimes v^*\otimes v\otimes v^* \end{smallmatrix} \right)\Big|_x, B \left( \begin{smallmatrix} u\otimes u^*\otimes u\otimes u^* \\ u\otimes u^*\otimes v\otimes v^* \\ v\otimes v^*\otimes v\otimes v^* \end{smallmatrix} \right)\Big|_y \right)_{\mathbb{C}^{3f^4}}$$

of a suitable matrix $B$, whose $3 \times 3$ block entries are of the form

$$B_{ij} = b_{ij} + \delta_{i,2}\delta_{j,2}\left(c_1\rho_1 + c_2\rho_2 + c_3\rho_3\right) \quad \text{with} \quad b_{ij}, c_i \in \mathbb{C},$$

and the operators $\rho_i$ permute the factors of the tensor product,

$$\begin{aligned}\rho_1(u\otimes u^*\otimes v\otimes v^*) &= v\otimes v^*\otimes u\otimes u^*\\ \rho_2(u\otimes u^*\otimes v\otimes v^*) &= u\otimes v^*\otimes v\otimes u^*\\ \rho_3(u\otimes u^*\otimes v\otimes v^*) &= v\otimes u^*\otimes u\otimes v^*\,.\end{aligned}$$

Hence introducing the operator

$$K\;:\;L^2(\mathcal{F},d\mu_L)\to\mathbb{C}^{3f^4}\;:\;\psi\mapsto\int_{\mathcal{F}}\begin{pmatrix}u\otimes u^*\otimes u\otimes u^*\\ u\otimes u^*\otimes v\otimes v^*\\ v\otimes v^*\otimes v\otimes v^*\end{pmatrix}\Big|_x\psi(x)\,d\mu(x)\,,$$

we find that $\mathcal{D}_\mu = K^*BK$. This gives the claim. □

In view of this lemma, we may decompose $\mathcal{D}$ in the form (6.4.13).

Using the U($f$)-invariance of $\mu$, the constant function $1_{\mathcal{F}}$ is a eigenfunction to the eigenvalue $\nu_0$

$$\nu_0 = (\nu_0 1_{\mathcal{F}})(x) = (\mathcal{D}_\mu 1_{\mathcal{F}})(x) = \int_{\mathcal{F}}\mathcal{D}(x,y)d\mu(y).$$

**Proposition 8.12.** *The eigenvalue $\nu_0$ in the decomposition* (6.4.13) *is given by*

$$\nu_0 = \frac{1}{f(f^2-1)}\Big((f-1)\alpha^4-2(f-1)\alpha^3\beta-6\alpha^2\beta^2-2(f-1)\alpha\beta^3+(f-1)\beta^4\Big). \quad (8.7.26)$$

*Proof.* Let $f\geq 3$. For elements $x,y\in\mathcal{F}$ given by (8.4.11), the eigenvalue $\nu_0$ is

$$\begin{aligned}\nu_0 = &\int_{-\infty}^{\infty}d\kappa\int_0^\infty dp\,p^2\,\mu(\kappa,p)\Theta(p-\kappa)\Theta(p+\kappa)\Theta(\beta+p-\kappa)\Theta(\alpha-p-\kappa)\\ &\times\int_0^{2\pi}d\varphi\int_0^\pi d\vartheta\,\sin\vartheta\,\mathcal{D}(\vartheta).\end{aligned}$$

Calculating the $\vartheta$-integral

$$\int_0^\pi d\vartheta\,\sin\vartheta\,\mathcal{D}(\vartheta) = \kappa^2(\alpha+\beta)^2+\frac{1}{3}p^2\left(\alpha^2-10\alpha\beta+\beta^2\right)$$

and using formula (8.5.21), we obtain after substituting $p+\kappa=\alpha s$ and $p-\kappa=\beta t$

$$\begin{aligned}\nu_0 =&\frac{(f-1)(f-2)^2}{6(\alpha+\beta)}\int_0^1 ds\int_0^1 dt\,\Big((1-s)(1-t)\Big)^{f-3}\\ &\times\Big((s^3\alpha^3+t^3\beta^3)(\alpha^2-\alpha\beta+\beta^2)-9\,s\,t\,\alpha^2\,\beta^2\,(s\alpha+t\beta)\Big)\\ =&\frac{(f-1)(f-2)^2}{6(\alpha+\beta)}\Big((\alpha^3+\beta^3)(\alpha^2-\alpha\beta+\beta^2)B(4,f-2)B(1,f-2)\\ &-9\alpha^2\beta^2(\alpha+\beta)B(3,f-2)B(2,f-2)\Big).\end{aligned}$$

Expressing the Beta function with the Γ-function and using the properties of the Γ-function we finally calculate

$$\begin{aligned}\nu_0 &= \tfrac{(f-1)(f-2)^2}{6}\Big((\alpha^2-\alpha\beta+\beta^2)^2\frac{\Gamma(4)\,\Gamma(f-2)^2}{\Gamma(f+2)\Gamma(f-1)} - 9\alpha^2\beta^2\frac{\Gamma(3)\Gamma(f-2)^2}{\Gamma(f+1)\Gamma(f)}\Big)\\ &= \frac{(f-1)(f-2)^2\Gamma(f-2)^2}{\Gamma(f+1)\,\Gamma(f-1)}\Big(\frac{(\alpha^2-\alpha\beta+\beta^2)^2}{f+1} - 3\alpha^2\beta^2\frac{1}{f-1}\Big)\\ &= \frac{1}{f}\left(\frac{\alpha^4-2\alpha^3\beta-2\alpha\beta^3+\beta^4}{f+1} - \frac{6\alpha^2\beta^2}{f^2-1}\right).\end{aligned}$$

A transformation yields formula (8.7.26). □

We discuss the obtained value of $\nu_0$: In the case $f=2$, one calculates

$$\nu_0 = \frac{1}{4\pi}\int_0^{2\pi} d\varphi \int_0^{\pi} d\vartheta \sin(\vartheta)\mathcal{D}(\vartheta),$$

which fits with formula (8.7.26) setting $f=2$.

In the limit $\beta \to 0$, we obtain formula (8.2.8), and consequently the minimal action of the variational principle. Using the eigenvalues $1\pm\tau$, one obtains

$$\nu_0 = \frac{2(3f+6f\tau^2-(2+f)\tau^4-6)}{f(f^2-1)}\,. \tag{8.7.27}$$

Unfortunately, the eigenvalue $\nu_0$ cannot be used as a lower bound since the operator $\mathcal{D}_\mu$ is not positive semi-definite:

**Lemma 8.13.** *If $f \geq 3$ and $\tau > 1$, the operator $\mathcal{D}_\mu$ has negative eigenvalues.*

*Proof.* Since $\operatorname{supp}\mu = \mathcal{F}$, it suffices to find two points $x_1, x_2 \in \mathcal{F}$ such that the corresponding Gram matrix $\mathcal{D}(x_i, x_j)$ is not positive semi-definite.
Let $\alpha \geq \beta$. We choose the four vectors

$$u_1 = e_1\,, \quad v_1 = e_2 \quad \text{and} \quad u_2 = e_1\,, \quad v_2 = e_3$$

(where $e_i$ are the standard basis vectors of $\mathbb{C}^f$). Taking the representation (3.2.14), we obtain two points $x_1, x_2 \in \mathcal{F}$. The corresponding Gram matrix is using (8.4.12) computed to be

$$\begin{pmatrix} \frac{1}{2}(\alpha^2-\beta^2)^2 & \frac{1}{2}\alpha^4 \\ \frac{1}{2}\alpha^4 & \frac{1}{2}(\alpha^2-\beta^2)^2 \end{pmatrix}.$$

The determinant of this matrix is negative.
In the case $\alpha < \beta$, we choose

$$u_1 = e_1\,, \quad v_1 = e_2 \quad \text{and} \quad u_2 = e_3\,, \quad v_2 = e_2,$$

yielding a Gramian whose determinant is negative. □

We conclude that Proposition 6.15 cannot be applied. With regard to Example 7.8 on the circle, the value $\nu_0$ can not be used for estimating the minimal action. This proof also shows that the operator $\mathcal{L}_\mu$ has negative eigenvalues, thus $\mu$ cannot be a minimizer.

## 8.8 The Structure of Minimizers

We now apply our main Theorems 6.19 and 6.21 to the family of matrices with prescribed eigenvalues. To simplify the notation, we again choose $\alpha, \beta$ as $\tau \pm 1$ for $\tau \geq 1$. We obtain the following general result.

**Theorem 8.14.** *Every minimizer $\rho$ on $\mathcal{F}_{1,2}(\mathbb{C}^f)$ is either generically timelike or satisfies $\overset{\circ}{\operatorname{supp}}\, \rho = \varnothing$.*

*Proof.* As a homogeneous space, the flag manifold $\mathcal{F}_{1,2}(\mathbb{C}^f)$ has a even real analytic structure (see [18, Chapter II, §4]). The function $\mathcal{D}$ is obviously real analytic. Moreover, it is symmetric and constant on the diagonal. In order to apply Theorem 6.19, for given $y \in \mathcal{K}(x)$ we must find a curve $c$ joining $x$ and $y$ which satisfies (6.5.17). Alternatively, in order to apply Theorem 6.21, our task is to construct a curve $c(t)$ with $c(0) = x$ and $c(1) = y$ which is analytic in a neighborhood of $t = 0$, such that the function $\mathcal{D}(c(t), y)$ changes sign at $t = 0$. Since in the case $\tau = 1$, the sets $\mathcal{K}(x)$ are all empty, we may assume that $\tau > 1$. We denote the range of $x$ by $I \subset \mathbb{C}^f$ and the orthogonal projection to $I$ by $\pi_I$. Choosing an orthonormal basis $(e_1, e_2)$ of $I$, the matrix $x|_I$ can according be represented by

$$x|_I = \mathbb{1}_2 + \tau\, \vec{u} \cdot \vec{\sigma} \qquad \text{with } \vec{u} \in S^2 .$$

(We remark that it may be $\vec{u} \neq \vec{e}_3$.) Similarly, the operator $\tilde{y} := \pi_I y \pi_I$ has the representation

$$\tilde{y}|_I = \kappa \mathbb{1}_2 + p\, \vec{v} \cdot \vec{\sigma} \qquad \text{with } \vec{v} \in S^2 ,$$

where the real parameters $\kappa$ and $p$ satisfy according to (8.4.15) the inequalities

$$1 - \tau \leq \kappa - p \leq 0 \leq \kappa + p \leq 1 + \tau .$$

The function $\mathcal{D}$ is given by (8.4.18) where now $\vartheta$ denotes the angle between $\vec{u}$ and $\vec{v}$ and the set $\mathcal{K}(x)$ is again given by (8.4.19).

The operator $\tilde{y}$ has rank two if and only if $p > |\kappa|$. A short calculation shows that in this case, $\mathcal{D}$ only has transverse zeros. Thus we can choose a direction $\dot{c}(0)$ where the condition (6.5.17) is satisfied. Choosing a smooth curve starting in this direction which joins $x$ and $y$, we can apply Theorem 6.19 (A) to conclude the proof in this case.

It remains to consider the situation when $\tilde{y}$ has rank at most one. This leads us to several cases. We begin with the case when $\tilde{y}|_I$ vanishes. In this case, we may restrict attention to the four-dimensional subspace $U = \operatorname{Im} x \oplus \operatorname{Im} y$. In a suitable basis $(e_1, \ldots, e_4)$ of this subspace, the operators $x$ and $y$ have the matrix representations

$$x = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes (\mathbb{1} + \tau\, \vec{u} \cdot \vec{\sigma}) , \qquad y = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes (\mathbb{1} + \tau\, \vec{v} \cdot \vec{\sigma}) ,$$

where again $\vec{u}, \vec{v} \in S^2$. With regard to (3.1.6), a unitary transformation of the basis vectors $e_1$ and $e_2$ describes a rotation of the vector $\vec{u}$ in $\mathbb{R}^3$. By a suitable trans-

formation of this type, we can arrange that the angle between $\vec{u}$ and $\vec{v}$ equals $\vartheta_{\max}$ (see (5.1.11)). We now define the curve $c : [0, \pi] \to \mathcal{F}_{1,2}(\mathbb{C}^f)$ by

$$c(t) = \begin{pmatrix} \cos(t)^2 & \sin(t)\cos(t) \\ \sin(t)\cos(t) & \sin(t)^2 \end{pmatrix} \otimes (\mathbb{1} + \tau\, \vec{w}(t) \cdot \vec{\sigma}), \tag{8.8.28}$$

where $\vec{w} : [0, \pi] \to S^2$ is the geodesic on $S^2$ with $\vec{w}(0) = \vec{u}$ and $\vec{w}(\pi) = \vec{v}$. The curve $c$ is a real analytic function with $c(0) = x$ and $c(\pi) = y$, which is obviously translation symmetric. Furthermore, one computes

$$\mathcal{D}(c(t), y) = \sin(t)^4\, \mathcal{D}_{S^2}(\vec{w}(t), \vec{v}),$$

where $\mathcal{D}_{S^2}$ is the corresponding function on the unit sphere (5.1.10). As $\mathcal{D}_{S^2}(\vartheta)$ changes sign at $\vartheta_{\max}$, the function $\mathcal{D}(c(t), y)$ changes sign at $t = 0$. Thus Theorem 6.21 (A) applies, completing the proof in the case $\tilde{y}|_I = 0$.

We next consider the case that $\tilde{y}$ has rank one. We choose the basis $(e_1, e_2)$ of $I$ such that $\tilde{y}$ is diagonal,

$$\tilde{y}|_I = \begin{pmatrix} a & 0 \\ 0 & 0 \end{pmatrix} \qquad \text{with } a \neq 0.$$

If the vector $(y - a)e_1$ is non-zero, we choose $e_3$ equal to a multiple of this vector. An elementary consideration shows that $y$ is invariant on the subspace $\langle\{e_1, e_2, e_3\}\rangle$ and can be written as

$$y|_{\langle\{e_1,e_2,e_3\}\rangle} = \begin{pmatrix} a & 0 & \overline{b} \\ 0 & 0 & 0 \\ b & 0 & c \end{pmatrix}. \tag{8.8.29}$$

If on the other hand $(y-a)e_1 = 0$, then $e_1$ is an eigenvector of $y$, and by choosing $e_3$ to be the other non-trivial eigenvector, $y|_{\langle\{e_1,e_2,e_3\}\rangle}$ is again of the form (8.8.29) (but now with $b = 0$). We let $U$ be the unitary transformation

$$U(t) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos t & \sin t \\ 0 & -\sin t & \cos t \end{pmatrix}.$$

Setting $y(t) = U(t)\, y\, U(t)^{-1}$, the matrix $\tilde{y}$ becomes

$$\tilde{y}(t) = \begin{pmatrix} 1 & 0 \\ 0 & \sin t \end{pmatrix} (\kappa\, \mathbb{1} + p\, \vec{v} \cdot \vec{\sigma}) \begin{pmatrix} 1 & 0 \\ 0 & \sin t \end{pmatrix},$$

where $\kappa$ and $p$ are new parameters with

$$p \geq |\kappa| \qquad \text{and} \qquad \kappa + p\, v_3 = a \neq 0\,. \tag{8.8.30}$$

The function $\mathcal{D}$ is now computed by

$$\begin{aligned} \mathcal{D}(x, y(t)) &= \frac{1}{2} \operatorname{Tr}\big(x|_I\, \tilde{y}(t)\big)^2 - 2 \det\big(x|_I\, \tilde{y}(t)\big) \\ &= \frac{1}{2}\Big(\operatorname{Tr}\big(x|_I\, \tilde{y}(t)\big)^2 - 4\,(\tau^2 - 1)\,(p^2 - \kappa^2)\, \sin^2 t\Big). \end{aligned} \tag{8.8.31}$$

In order to simplify the trace, we transform the phase of $e_3$. This changes the phase of $b$ in (8.8.29), thus describing a rotation of the vector $\vec{v}$ in the $(1,2)$-plane. This makes it possible to arrange that the vectors $(u_1, u_2)$ and $(v_1, v_2)$ are orthogonal in $\mathbb{R}^2$. We thus obtain

$$\mathrm{Tr}\big(x|_I\, \tilde{y}(t)\big) = (1+\tau\, u_3)\,(\kappa + p\, v_3) + (1-\tau\, u_3)\,(\kappa - p\, v_3)\, \sin^2 t\,.$$

We now have two subcases:

(1) $v_3 \neq \pm 1$: We vary the vectors $\vec{u}$ and $\vec{v}$ as functions of $t$ such that the above orthogonality relations remain valid and

$$u_3 = \cos(\vartheta + \alpha\, t)\,, \qquad v_3 = \cos(\varphi + \beta\, t)$$

with free "velocities" $\alpha$ and $\beta$. Since $\mathcal{L}(x,y) = 0$ at $t = 0$, we know that

$$\cos\vartheta = -\frac{1}{\tau}\,, \qquad \sin\vartheta = \frac{\sqrt{\tau^2-1}}{\tau} \neq 0\,. \tag{8.8.32}$$

A Taylor expansion yields

$$\mathrm{Tr}\big(x|_I\, \tilde{y}(t)\big) = -t\,\alpha\tau\,(\kappa + p v_3)\, \sin\vartheta \tag{8.8.33}$$

$$+ \frac{t^2}{2}\Big((4+\alpha^2)\,\kappa + (-4+\alpha^2) p\cos\varphi + 2\alpha\beta p\tau\, \sin\vartheta\, \sin\varphi\Big) + \mathcal{O}(t^3)\,. \tag{8.8.34}$$

As the factor $(\kappa + p v_3)$ is non-zero in view of (8.8.30), the linear term (8.8.33) does not vanish whenever $\alpha \neq 0$. By suitably adjusting $\alpha$, we can arrange that the square of this linear term compensates the last term in (8.8.31) (which is also non-zero in view of our assumption $p > \kappa$). Next, we know from (8.8.32) and our assumptions that the term $\sim \alpha\beta$ in (8.8.34) is non-zero. Thus by a suitable choice of $\beta$, we can give the quadratic term (8.8.34) any value we want. Taking the square, in (8.8.31) we get a contribution $\sim t^3$. Thus the function $\mathcal{D}$ changes sign. Transforming to a suitable basis where $y$ is a fixed matrix, we obtain a curve $x(t)$ which is locally translation symmetric. Extending this curve to a smooth curve $c$ which joins the point $y$, we can apply Theorem 6.21 (A).

(2) $v_3 = \pm 1$: We know that the matrix $\tilde{y}$ is diagonal,

$$\tilde{y}(t) = \begin{pmatrix} \kappa \pm p & 0 \\ 0 & (\kappa \mp p)\sin^2 t \end{pmatrix}\,. \tag{8.8.35}$$

Now we keep $v$ fixed, while we choose the curve $u(t)$ to be a great circle which is inclined to the $(1,3)$-plane by an angle $\gamma \neq 0$, i.e.

$$u_3 = \cos(\vartheta + \alpha t)\, \cos\gamma\,.$$

Repeating the above calculation leading to (8.8.33) and (8.8.34), one sees that we again get a non-zero contribution to $\mathcal{D}$ of the order $\sim t^3$. Thus $\mathcal{D}$ again

changes sign, making it possible to apply Theorem 6.21 (A). It remains to consider the case when $\tilde{y}$ vanishes but $y|_I \neq 0$. A short calculation shows that $y|_I$ cannot have rank two. Thus we can choose the orthonormal basis $(e_1, e_2)$ of $I$ such that $ye_1 \neq 0$ and $ye_2 = 0$. By suitable extending this orthonormal system by $e_3$ and $e_4$, we can arrange that the operator $y$ is invariant on the subspace $\langle\{e_1, e_2, e_3, e_4\}\rangle$ and has the matrix representation

$$y_{\langle\{e_1,e_2,e_3,e_4\}\rangle} = \begin{pmatrix} 0 & 0 & \overline{a} & 0 \\ 0 & 0 & 0 & 0 \\ a & 0 & c & \overline{b} \\ 0 & 0 & b & 0 \end{pmatrix}.$$

If $b \neq 0$, we can again work with the curve (8.8.28). If on the other hand $b = 0$, the operator $y$ is invariant on $\langle\{e_1, e_2, e_3\}\rangle$ and has the canonical form

$$y_{\langle\{e_1,e_2,e_3\}\rangle} = \begin{pmatrix} 0 & 0 & \sqrt{\tau^2 - 1} \\ 0 & 0 & 0 \\ \sqrt{\tau^2 - 1} & 0 & 0 \end{pmatrix}.$$

Transforming $y$ by the unitary matrix

$$V(\tau) \begin{pmatrix} e_1 \\ e_3 \end{pmatrix} = \begin{pmatrix} \cos\tau & \sin\tau \\ -\sin\tau & \cos\tau \end{pmatrix} \begin{pmatrix} e_1 \\ e_3 \end{pmatrix},$$

we can arrange that $y$ is again of the form (8.8.29), but now with coefficients depending on $\tau$. Setting $t = \tau^2$, we can again use the construction after (8.8.29). This completes the proof.

□

For sufficiently large $\tau$, we can rule out one of the cases in Theorem 8.14, showing that the minimizing measures do have a singular support.

**Theorem 8.15.** *There are no generically timelike minimizers if*

$$\tau^2 > \frac{3f + 2\sqrt{3\,(f^2 - 1)}}{(2 + f)}.$$

The method of proof is to apply Proposition 6.17 (I) on the eigenvalue $\nu_0$ given by (8.7.27).

The remaining question is whether generically timelike minimizers exist for small $\tau$. In the special case $\tau = 1$, according to Proposition 8.4 the homogenizer $\mu$ is a generically timelike minimizer. If $\tau > 1$, the propositions 6.6 and 6.15 can no longer be used, because the operator $D_\mu$ fails to be positive semi-definite, as shown in Lemma 8.13. In this situation, Proposition 6.18 still gives some information on the possible support of generically timelike minimizers. In the final Section, we will conjecture that only if $\tau = 1$ generically timelike minimizers exist.

## 8.9 Spherical Solutions for an Even Number of Particles

In the case that $f$ is an even number, it is possible to assign to a vector on the two-sphere an element in $\mathcal{F}$ as we now describe. The variational principle restricted on the obtained subset of $\mathcal{F}$ can then be regarded as a variational principle on the sphere, and the minimal action will yield an upper bound of the original variational principle on the flag manifold.
To this purpose, we study the already used spherical harmonics in more detail: For integer $l > 0$ and $m = -l, \dots, l$ the spherical harmonics are explicitly given by

$$Y_{l,m}(\vartheta, \varphi) = \frac{(-1)^l}{2^l l!} \sqrt{\frac{(2l+1)!\,(l+m)!}{4\pi(2l)!\,(l-m)!}}\, e^{im\varphi}\, \sin^{-m}\vartheta \frac{d^{l-m}}{d(\cos\vartheta)^{l-m}} \sin^{2l}\vartheta. \quad (8.9.36)$$

If $\vec{L}$ denotes the angular momentum operator, expressed in spherical coordinates, for fixed $l \in \mathbb{N}$ and $m = -l, \dots, l$, the functions $Y_{l,m}$ are the $2l+1$ eigenfunctions of $L^2$ to the eigenvalue $l(l+1)$ (setting $\hbar = 1$). We refer to [26, Chapter 5] for the properties of the induced objects. In the following evaluations, we use the value of the spherical harmonics on the north pole.

**Lemma 8.16.** *On the north pole, the spherical harmonics are evaluated as*

$$Y_{l,0}(0,0) = \sqrt{\frac{2l+1}{4\pi}}, \;\; Y_{l,m}(0,0) = 0 \;\; \textit{for all} \;\; m \in \{-l, \dots, l\} \backslash \{0\}. \quad (8.9.37)$$

*Proof.* The Leibniz rule yields

$$\tfrac{d^{l-m}}{d(\cos\vartheta)^{l-m}}(1-\cos^2\vartheta)^l = \sum_{\nu=0}^{l-m} \binom{l-m}{\nu} (-1)^\nu \tfrac{l!}{(l-\nu)!} (1-\cos\vartheta)^{l-\nu} \tfrac{l!}{(m+\nu)!} (1+\cos\vartheta)^{m+\nu}.$$

Inserting in (8.9.36), we obtain $Y_{l,m}(0,0) \neq 0$ if and only if $m = 0$. □

Now let $l \in \mathbb{N}$ be fixed. We introduce the *spin spherical harmonics* which are defined as the two component wave functions

$$\varphi_m(\vec{x}) = \begin{pmatrix} \sqrt{\frac{l+1/2+m}{2l+1}}\, Y_{l,m-\frac{1}{2}}(\vec{x}) \\ \sqrt{\frac{l+1/2-m}{2l+1}}\, Y_{l,m+\frac{1}{2}}(\vec{x}) \end{pmatrix} \quad \text{for} \quad \vec{x} \in S^2$$

for $m = \pm\frac{1}{2}, \dots, \pm(l+\frac{1}{2})$, see [27, Chapter 8]. These are the $2l+2$ eigenfunctions of the total angular momentum $\vec{L} \cdot \vec{\sigma}$ corresponding to the eigenvalue $l$.

**Lemma 8.17.** *Let $\Pi_l$ be the projector onto the eigenspace of the operator $\vec{L} \cdot \vec{\sigma}$, thus*

$$\Pi_l(\vec{x}, \vec{y}) = \sum_{m=-(l+1/2)}^{l+1/2} \varphi_m(\vec{x}) \varphi_m(\vec{y})^\dagger \quad \textit{for} \quad \vec{x}, \vec{y} \in S^2.$$

*Then for each $R \in SO(3)$ there exists a unique $V \in SU(2)$ such that*

$$\Pi_l(R\,\vec{x}, R\,\vec{y}) = V\,\Pi_l(\vec{x},\vec{y})\,V^{-1} \quad \text{for all} \quad \vec{x},\vec{y} \in S^2. \tag{8.9.38}$$

*In particular,*

$$\Pi_l(\vec{x},\vec{x}) = \frac{l+1}{4\pi}\,\mathbb{1}_2 \quad \text{for all} \quad \vec{x} \in S^2. \tag{8.9.39}$$

*Proof.* The first statement follows from the fact that the operator $\vec{L}\cdot\vec{\sigma}$ is spherically symmetric and that $\mathrm{SO}(3) \simeq \mathrm{SU}(2)/\{\pm 1\}$. In order to calculate $\Pi_l(\vec{x},\vec{x})$, we can consequently choose $\vec{x} = \vec{e_3}$, and use formula (8.9.37). □

With this Lemma, we can construct a mapping on the family of matrices with prescribed eigenvalues:

**Proposition 8.18.** *Let $a, b \in \mathbb{R}$ and $\vec{x} \in S^2$. Then $F(\vec{x}) \in \mathrm{Mat}\big((2l+2)\times(2l+2), \mathbb{C}\big)$ defined as*

$$F(\vec{x}) = \Big( \big(\varphi_m(\vec{x}) \big| (a\,\mathbb{1}_2 + b\,\vec{x}\cdot\vec{\sigma})\varphi_n(\vec{x})\big)_{\mathbb{C}^2} \Big)_{m,n=-(l+1/2),\ldots,(l+1/2)} \tag{8.9.40}$$

*is hermitian of rank at most two. Its non-vanishing eigenvalues are given by*

$$\frac{l+1}{4\pi}\,(a \pm b). \tag{8.9.41}$$

*Proof.* According to Formula (8.9.40), the matrix $F = F(\vec{x})$ is hermitian with $\mathrm{rk}(F) \leq 2$. Using the invariance of the trace under cyclic permutations and formula (8.9.39), we obtain

$$\mathrm{Tr}(F) = \mathrm{Tr}\big((a\,\mathbb{1}_2 + b\,\vec{x}\cdot\vec{\sigma})\,\Pi_l(\vec{x},\vec{x})\big) = \frac{l+1}{4\pi}\mathrm{Tr}(a\,\mathbb{1}_2 + b\,\vec{x}\cdot\vec{\sigma}) = \frac{l+1}{2\pi}a$$

and

$$\begin{aligned}\mathrm{Tr}(F^2) &= \mathrm{Tr}\big((a\,\mathbb{1}_2 + b\,\vec{x}\cdot\vec{\sigma})\,\Pi_l(\vec{x},\vec{x})\,(a\,\mathbb{1}_2 + b\,\vec{x}\cdot\vec{\sigma})\,\Pi_l(\vec{x},\vec{x})\big) \\ &= \big(\tfrac{l+1}{4\pi}\big)^2\,\mathrm{Tr}(a^2\,\mathbb{1}_2 + ab\,\vec{x}\cdot\vec{\sigma} + b^2\,\mathbb{1}_2) = \big(\tfrac{l+1}{4\pi}\big)^2\,(2a^2+2b^2),\end{aligned}$$

concluding that the non-vanishing eigenvalues of $F$, which are uniquely determined by $\mathrm{Tr}(F)$ and $\mathrm{Tr}(F^2)$, are independent of $\vec{x}$. □

We apply this Proposition to obtain a subset of $\mathcal{F}$ in the case $f = 2(l+1)$. Thus we demand that the eigenvalues of $F(\vec{x})$ are given by $\alpha$ and $-\beta$. According to (8.9.41), we determine the real parameters $a, b$ by

$$a = \frac{2\pi}{l+1}(\alpha - \beta), \quad b = \frac{2\pi}{l+1}(-\alpha - \beta). \tag{8.9.42}$$

The function $\mathcal{D}$ and thus the Lagrangian restricted on the subset $\{F(\vec{x}) \,:\, \vec{x} \in S^2\}$ can be regarded as a function on $S^2 \times S^2$. Let

$$\mathcal{D}_S : S^2 \times S^2 \to \mathbb{R}, \quad \mathcal{D}_S(\vec{x},\vec{y}) = \mathcal{D}(F(\vec{x}), F(\vec{y})),$$

where $\mathcal{D}$ is the function on $\mathcal{F}$ defined in (8.3.10).

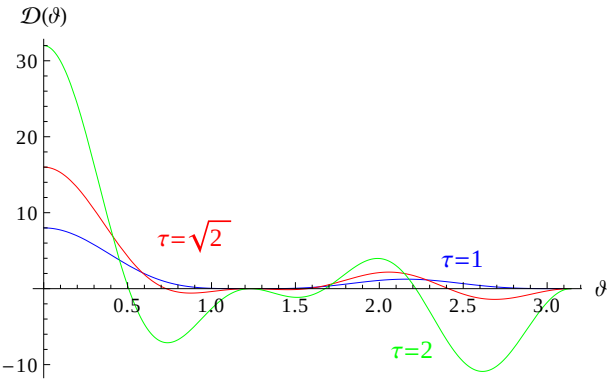



Figure 8.3: The function $\mathcal{D}$ in the spheric symmetric setting.

**Lemma 8.19.** *The function $\mathcal{D}_S(\vec{x},\vec{y})$ just depends on the angle $\vartheta \in [0,\pi]$ given by $\cos(\vartheta) = \vec{x}\cdot\vec{y}$ between the points $\vec{x},\vec{y} \in S^2$.*

*Proof.* Let $R \in \mathrm{SO}(3)$. Since $\mathrm{SO}(3) \simeq \mathrm{SU}(2)/\{\pm\mathbb{1}_2\}$, there exists a unique unitary matrix $V \in \mathrm{SU}(2)$ such that both formulas (3.1.6) and (8.9.38) are satisfied. We obtain

$$\begin{aligned}\mathrm{Tr}\big(F(R\vec{x})F(R\vec{y})\big) &= \mathrm{Tr}\big((a+b\,(R\vec{x})\cdot\vec{\sigma})\,\Pi_l(R\vec{x},R\vec{y})\,(a+b\,(R\vec{y})\cdot\vec{\sigma})\,\Pi_l(R\vec{y},R\vec{x})\big)\\ &= \mathrm{Tr}\big(V(a+b\,(\vec{x})\cdot\vec{\sigma})\,\Pi_l(\vec{x},\vec{y})\,(a+b\,(\vec{y})\cdot\vec{\sigma})\,\Pi_l(\vec{y},\vec{x})V^{-1}\big)\\ &= \mathrm{Tr}\big(F(\vec{x})F(\vec{y})\big).\end{aligned}$$

Similarly, one obtains $\mathrm{Tr}\big((F(R\vec{x})F(R\vec{y}))^2\big) = \mathrm{Tr}\big((F(\vec{x})F(\vec{y}))^2\big)$. We conclude that $\mathcal{D}(F(R\vec{x}),F(R\vec{y})) = \mathcal{D}(F(\vec{x}),F(\vec{y}))$. □

For the calculation of the function $\mathcal{D}_S(\vec{x},\vec{y})$, we can consequently assume that $\vec{x} = \vec{e}_3$ and $\vec{y} \in S^2$ is arbitrary.

The minimizer of the variational principle on $S^2$ with respect to the function $\mathcal{D}_S$ yields an upper bound on the minimal action $\mathcal{S}_{\min}$ of the variational principle on the whole flag manifold $\mathcal{F}$,

$$\inf_{\rho\in\mathfrak{M}(\mathcal{F})} \mathcal{S}[\rho] \leq \inf_{\rho\in\mathfrak{M}(S^2)} \mathcal{S}[\rho].$$

Exemplarily, we now consider the case $f = 4$ resp. $l = 1$. We again prescribe the eigenvalues $\alpha, -\beta$ as $1\pm\tau$ for $\tau \geq 1$. In this case, the function $\mathcal{D}_S$ is calculated as

$$\mathcal{D}_S(\vartheta) = \tfrac{1}{8}\tau^2(1+\cos\vartheta)(1-3\cos\vartheta)^2\Big(2(1+3\cos^2\vartheta)+\tau^2(\cos\vartheta-1)(1+3\cos\vartheta)^2\Big) \tag{8.9.43}$$

Typical plots are shown in Figure 8.3. This example differs from the already examined examples on the sphere in its causal structure. If $\tau > 1$, the function $\mathcal{D}_S$ has five zeros, namely at $\vartheta = \arccos(1/3)$, $\vartheta = \pi$ and the three zeros of the polynomial term

$$\left(9\tau^2\cos^3\vartheta - 3\left(\tau^2-2\right)\cos^2\vartheta - 5\tau^2\cos\vartheta - \tau^2 + 2\right),$$

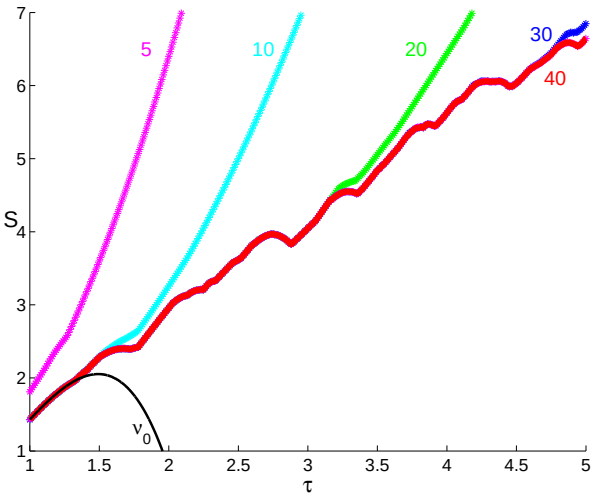



Figure 8.4: Numerical minima for the weighted counting measure on the circle.

denoted in ascending order as $\vartheta_1 < \arccos(1/3) < \vartheta_2 < \arccos(-1/3) < \vartheta_3$. In particular, for all $\tau \geq 1$ it is $\mathcal{D}_S(\arccos(-1/3)) = \frac{8}{9}\tau^2 > 0$. The light-cones are given as

$$\begin{aligned}
\mathcal{I}(x) &= \big\{ y \in S^2 : x \cdot y \in (-1, \cos\vartheta_3) \cup \big(\cos\vartheta_2, \tfrac{1}{3}\big) \cup \big(\tfrac{1}{3}, \cos\vartheta_1\big) \big\}, \\
\mathcal{J}(x) &= \big\{ y \in S^2 : x \cdot y \in [-1, \cos\vartheta_3] \cup [\cos\vartheta_2, \cos\vartheta_1] \big\}, \\
\mathcal{K}(x) &= \{ y \in S^2 \;:\; x \cdot y = \cos\vartheta_3 \text{ or } x \cdot y = \cos\vartheta_2 \text{ or } x \cdot y = \cos\vartheta_1 \}.
\end{aligned}$$

For a better understanding, we first consider the variational principle on the circle. Using the same numerical routine as in Section 7.1, we obtain the results shown in Figure 8.4. We now apply the structural results of Chapter 6. Let $\mu$ again denote the Lebesgue measure on the circle. The eigenvalues of the operator $\mathcal{D}_\mu$ are calculated in general as

$$\nu_k = \frac{1}{2\pi} \int_0^{2\pi} \cos(k\vartheta) \mathcal{D}_S(\vartheta) d\vartheta \quad \text{for} \quad k \in \mathbb{N}. \tag{8.9.44}$$

The eigenvalue corresponding to the constant function, given by

$$\nu_0 = \frac{1}{128} \tau^2 \left(236 - 53\tau^2\right), \tag{8.9.45}$$

is positive for $\tau \in [1, 2\sqrt{\frac{59}{53}}]$. In this range, it is and $\nu_1, \ldots, \nu_6 > 0$, $\nu_k = 0$ for $k > 6$. Applying Proposition 6.17, there cannot exist generically timelike minimizers if $\tau > 2\sqrt{\frac{59}{53}} \approx 2.11017$. The measure supported at the set $X_8$ given by (7.1.1) with equal weights is a generically timelike minimizer for $\tau < \left[1, 2\sqrt{\frac{5}{10+\sqrt{2}}}\right]$. Proposition 6.15 yields that in this range every minimizer is generically timelike. The numerics show that indeed the generically timelike minimizer is for $\tau \approx 1$ not unique, but a statement similar to Lemma 7.1 does not hold. If $\tau > 2\sqrt{\frac{5}{10+\sqrt{2}}}$, the numerics

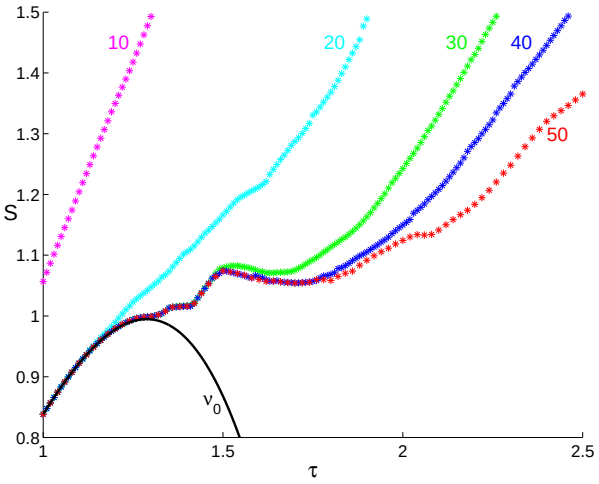



Figure 8.5: Numerical minima for the weighted counting measure on the sphere.

suggest that there does not exist a generically timelike minimizer. We assume that the critical value of $\tau$, where a phase transition occurs, is given as

$$\tau_c = 2\sqrt{\frac{5}{10+\sqrt{2}}} \approx 1.32371.$$

But a proof of this assumption lacks.

Theorem 6.19 yields that for $\tau > \tau_c$ it is $\operatorname{supp}^{\circ} \rho = \varnothing$. Additionally the numerics suggest that for each $x \in \operatorname{supp} \rho$ there exists $y \in \operatorname{supp} \rho \cap \mathcal{K}(x)$. The boundary $\mathcal{K}(x)$ consists of several orbits, but no orbit is stressed out. Thus it is not possible to define a chain as done in Definition 7.3.

We now consider the function $\mathcal{D}_S$ defined in (8.9.43) as a function on $S^2 \times S^2$, where for $x, y \in S^2$ we set $\cos\vartheta = x \cdot y$. The eigenvalues are now calculated in general as

$$\nu_k = \frac{1}{2} \int_0^\pi \mathcal{D}_S(\vartheta) P_k(\cos\vartheta) \sin\vartheta \, d\vartheta \quad \text{for} \quad k \in \mathbb{N}, \tag{8.9.46}$$

where $P_k$ denotes the $k$-th Legendre polynomial. The eigenvalue corresponding to the constant function, given by

$$\nu_0 = \tau^2 \left( \frac{6}{5} - \frac{38}{105} \tau^2 \right), \tag{8.9.47}$$

is positive for $\tau \in [1, 3\sqrt{\frac{7}{19}}]$. In this range, it is and $\nu_1, \ldots, \nu_6 > 0$, $\nu_k = 0$ for $k > 6$, concluding that there cannot exist generically timelike minimizers in the case $\tau > 3\sqrt{\frac{7}{19}} \approx 1.82093$. The numerical results have to be very precise in order to decide whether the minimizer is indeed generically timelike or not. But it seems that the critical value of $\tau$ now is different since the equality $\mathcal{S}_{\min} = \nu_0$ only holds

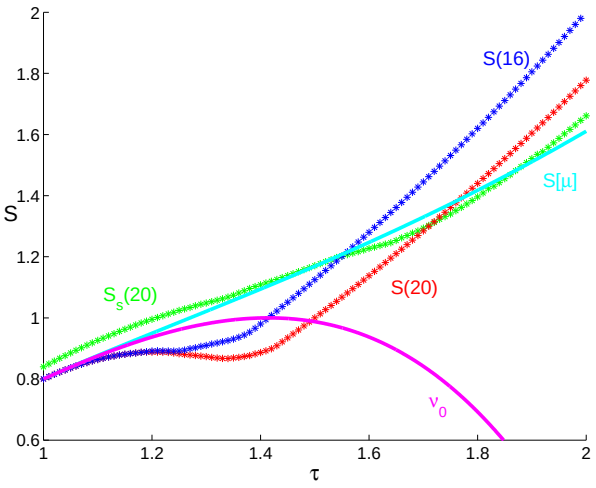



Figure 8.6: Numerical minima for the weighted counting measure on the flag manifold.

if $\tau < 1.1$, as can be seen in Figure 8.5. Additionally, the plots suggest that again the minimizing measure is a discrete measure supported at only a finite number of points.

## 8.10 Terminal Examination in Example

If the matrices are higher dimensional, an explicit construction and a more detailed study like we have made in Section 5.4 for small systems may not be possible. In this case, neither a distribution comparable to the Tammes distribution on the sphere is available nor a convenient method for constructing the Gramian is known.

To gain a first insight, we regard solutions of the variational principle on the flag manifold we obtained by using a local optimization routine in matlab. The method of simulated annealing is not appropriate because now the variational principle is a non-linear minimization problem with equality constraints, and thus cannot be solved using the simulated annealing algorithm. The solutions found using a local optimization routine may not be reasonable especially for larger systems, nevertheless can be used to state first predictions about the structural behavior.

We examine the minimizer calculated this way for $f = 4$, because in this case we can apply the considerations of the previous section and test the quality of the constructed upper bound. We again consider the case where the eigenvalues are given by $1 \pm \tau$. The obtained results are shown in Figure 8.6. We compare the numerical results with the minimizers of the variational principle according to the function $\mathcal{D}_S$ given by (8.9.43), with the upper bound $\mathcal{S}[\mu]$ calculated in Section 8.6 and with the eigenvalue $\nu_0$ given by (8.7.27). We make the following observations:

In the case $\tau = 1$, the minimal action coincides with $\nu_0$ and $\mathcal{S}[\mu]$ and is given by $\mathcal{S}_{\min} = 0.8$, compare Section 8.2. The minimizing measure supported at most at

16 points is a generically timelike minimizer. In the case $\tau > 1$ but close to 1, the numerics show that the minimizing measure supported at most at 16 points yields an action which is strictly smaller than the eigenvalue $\nu_0$. Thus the minimizing measure can not be generically timelike. We assume that only in the case $\tau = 1$ generically timelike minimizer exist. The minimal measure supported at most at 20 points coincides with the action of the minimal measure supported at most at 16 points. If the measure really is a global minimizer, we may deduce that the minimizing measure is supported at a finite number of points. If $\tau > 1.2$, the minimizing measure may be supported at more than 16 points.

Again increasing $\tau$, the numerical solutions can not be a global minimizer since both the minimizer of the variational principle according to the function $\mathcal{D}_S$ given by (8.9.43) and the action $\mathcal{S}[\mu]$ of the homogenizer yield a lower action.

We remark that the results for $f = 3$ behave qualitatively similar. Using the same routine in the case $f = 2$, we obtain the global minimizer if $\tau \leq \sqrt{2}$. If $\tau > \sqrt{2}$, the minimization routine stays in the local but no longer global minimum. Recalling the behavior if the function $\mathcal{S}$ shown in Figure 5.3, we may assume that for small $\tau$ the obtained results are reasonable.

To conclude, we state the final conjecture based on the numerical results:

**Conjecture 8.20.** *Consider the variational principle* (6.1.5) *corresponding to the function* $\mathcal{D}$ *given by* (8.3.10) *on the flag manifold* $\mathcal{F}_{1,2}(\mathbb{C}^f)$. *If* $f \geq 3$, *generically timelike minimizers exist only for* $\tau = 1$. *If* $\tau > 1$, *every minimizing measure is discrete with finite support.*

A satisfying numerical justification or a proof of this assumption is still outstanding.

# 9 Conclusions

The causal variational principles opened up striking mathematical structures despite the elementary and conceptual formulation. This work just treated the basic setting in small systems, where already fundamental effects appeared and features of physical importance displayed. Besides the symmetry breaking, and the arise of a causal structure, in the homogeneous setting a phase transition and a discrete structure, interpreted as first quantization, occurred. The fermionic projector induces structures spontaneously on the discrete space-time, which emphasize the fundamental nature of the object.

The homogeneous fermion systems yielded a wider class of general causal variational principles on measure spaces, whose minimizer could be characterized as generically timelike or singular. This effect is particularly noticeable as the variational principle does not have exceptional properties. The singularity is expressed weakly on the measure to have an empty interior. It would be highly desirable to show that the singular continuous part of the measure vanishes, and that the measure is a discrete measure supported at only a finite number of points, like the numerical solutions suggested.

For initial insights, our research efforts focused on variational principles of two particles, as its geometry is graphically accessible. We were able to prove most features and estimate the action from above and below. Increasing the number of particles and the number of space-time points, the systems become difficult to examine as a descriptive geometry model is lacking. We succeeded in applying the structural results, but the situation changes in comparison to two particle systems, as the light-cones of the causal system and the integral operators now have different properties.

For further studies on larger systems, it is necessary to develop new tools and theories. Given the simulated annealing algorithm we used fails for a constrained optimization problem, which class the variational principle on the flag manifold can be assigned, a next step could be to apply different global optimization algorithms. In order to understand what happens if the number of space-time points and particles tend to infinity, it might be gratifying to estimate the minimal action in the homogeneous setting analogous to systems of two particles, but the attempts of Section 7.2.2 may not be carried over in an obvious way, thus new estimation methods might have to be developed.

# A Code of Augmented Lagrangian Method

```
#include<stdio.h>
#include<math.h>
#include<stdlib.h>

#define f 2
#define m 5

double func(FILE *fd,double v[][f],double w[][f], double x[][f], double y[][f],double abl[],int Z
    );
int restr( double v[][f],double w[][f], double x[][f], double y[][f],double r[][f],double ablr[],
     double lambda[][f], double mu);
double cgmin(FILE *fd, double v[][f], double w[][f], double x[][f], double y[][f], double mu,
     double tau, double lambda[][f]);
int neu(double a, double v[][f], double w[][f], double x[][f], double y[][f], double va[][f],
     double wa[][f], double xa[][f], double ya[][f],double p[]);

int main (void)
{
   int i,j,k,l;
   double v[m][f],w[m][f],x[m][f],y[m][f],lambda[f][f],abl[4*m*f];
   double mu,R,funk,rho=1.2,gamma=0.4,tau=1.0E-10;
   FILE *fd;
   char *dateiname = "m5f2.txt";
   fd = fopen(dateiname, "w+");
   for(k=1;k<=20;k++)
   {
      for(i=0;i<m;i++)
      {
         for(j=0;j<f;j++)
         {
            v[i][j]=pow(-1,rand()%2)*(rand()%50)/100;
            w[i][j]=pow(-1,rand()%2)*(rand()%50)/100;
            x[i][j]=pow(-1,rand()%2)*(rand()%50)/100;
            y[i][j]=pow(-1,rand()%2)*(rand()%50)/100;
         }
      }
      for(i=0;i<f;i++)
      {
         for(j=0;j<f;j++)  lambda[i][j]=0;
      }
      l=1;mu=1000;R=1;tau=1.0E-10;
      while(R>1.0E-20 && l<200)
      {
         R=cgmin(fd,v,w,x,y,mu,tau,lambda);
         mu=mu*rho;
         tau=tau*gamma;
         l++;
      }
      fprintf(fd,"\n");
      func(fd,v,w,x,y,abl,1);
      funk=func(fd,v,w,x,y,abl,0);
      fprintf(fd,"%d\t%E\t",l,R);
   }
   return 0;
}

double func(FILE *fd,double v[][f],double w[][f], double x[][f], double y[][f],double abl[], int
    Z)
{
   int i,j,k,chi[m][m];
   double rtt[m][m]={{0}},itt[m][m]={{0}},rtu[m][m]={{0}},itu[m][m]={{0}},rut[m][m]={{0}},iut[m][
       m]={{0}},ruu[m][m]={{0}},iuu[m][m]={{0}};
   double tr[m][m],Re[m][m],Im[m][m],det[m][m],D[m][m];
   double funk=0;

   for(i=0;i<m;i++)
   {
      for(j=0;j<=i;j++)
      {
         for(k=0;k<f;k++)
         {
            rtt[i][j]+=v[i][k]*v[j][k]+w[i][k]*w[j][k];
            itt[i][j]+=w[i][k]*v[j][k]-v[i][k]*w[j][k];
            rtu[i][j]+=v[i][k]*x[j][k]+w[i][k]*y[j][k];
```

```
                itu[i][j]+=w[i][k]*x[j][k]-v[i][k]*y[j][k];
                rut[i][j]+=x[i][k]*v[j][k]+y[i][k]*w[j][k];
                iut[i][j]+=y[i][k]*v[j][k]-x[i][k]*w[j][k];
                ruu[i][j]+=x[i][k]*x[j][k]+y[i][k]*y[j][k];
                iuu[i][j]+=y[i][k]*x[j][k]-x[i][k]*y[j][k];
            }
        }
    }
    for(i=0;i<m;i++)
    {
        for(j=0;j<=i;j++)
        {
            tr[i][j]=rtt[i][j]*rtt[i][j]+itt[i][j]*itt[i][j]-
            rtu[i][j]*rtu[i][j]-itu[i][j]*itu[i][j]-rut[i][j]*rut[i][j]-iut[i][j]*iut[i][j]+ruu[i][j
                ]*ruu[i][j]+iuu[i][j]*iuu[i][j];
            Re[i][j]=rtt[i][j]*ruu[i][j]-itt[i][j]*iuu[i][j]-rtu[i][j]*rut[i][j]+itu[i][j]*iut[i][j
                ];
            Im[i][j]=itt[i][j]*ruu[i][j]+rtt[i][j]*iuu[i][j]-itu[i][j]*rut[i][j]-rtu[i][j]*iut[i][j
                ];
            det[i][j]=Re[i][j]*Re[i][j]+Im[i][j]*Im[i][j];
            D[i][j]=tr[i][j]*tr[i][j]-4*det[i][j];
            if(D[i][j]>=0) chi[i][j]=1;
                    else chi[i][j]=0;
        }
    }
    for(i=0;i<m;i++)
    {
            for(j=0;j<i;j++) funk=funk+chi[i][j]*D[i][j];
            funk=funk+0.5*D[i][i];
    }
    for(i=0;i<4*m*f;i++) abl[i]=0;
    for(i=0;i<m;i++)
    {
        for(j=0;j<i;j++)
        {
            if(chi[i][j]==1)
            {
                for(k=0;k<f;k++)
                {
                    abl[f*i+k]+=4*tr[i][j]*(rtt[i][j]*v[j][k]-itt[i][j]*w[j][k]-rtu[i][j]*x[j][k]+itu[
                        i][j]*y[j][k])-8*(Re[i][j]*(v[j][k]*ruu[i][j]+w[j][k]*iuu[i][j]-x[j][k]*rut[i
                        ][j]-y[j][k]*iut[i][j])+Im[i][j]*(-w[j][k]*ruu[i][j]+v[j][k]*iuu[i][j]+y[j][k
                        ]*rut[i][j]-x[j][k]*iut[i][j]));
                    abl[f*j+k]+=4*tr[i][j]*(rtt[i][j]*v[i][k]+itt[i][j]*w[i][k]-rut[i][j]*x[i][k]-iut[
                        i][j]*y[i][k])-8*(Re[i][j]*(v[i][k]*ruu[i][j]-w[i][k]*iuu[i][j]-x[i][k]*rtu[i
                        ][j]+y[i][k]*itu[i][j])+Im[i][j]*(w[i][k]*ruu[i][j]+v[i][k]*iuu[i][j]-x[i][k
                        ]*itu[i][j]-y[i][k]*rtu[i][j]));
                    abl[m*f+f*i+k]+=4*tr[i][j]*(rtt[i][j]*w[j][k]+itt[i][j]*v[j][k]-rtu[i][j]*y[j][k]-
                        itu[i][j]*x[j][k])-8*(Re[i][j]*(w[j][k]*ruu[i][j]-v[j][k]*iuu[i][j]-y[j][k]*
                        rut[i][j]+x[j][k]*iut[i][j])+Im[i][j]*(v[j][k]*ruu[i][j]+w[j][k]*iuu[i][j]-x[
                        j][k]*rut[i][j]-y[j][k]*iut[i][j]));
                    abl[m*f+f*j+k]+=4*tr[i][j]*(rtt[i][j]*w[i][k]-itt[i][j]*v[i][k]-rut[i][j]*y[i][k]+
                        iut[i][j]*x[i][k])-8*(Re[i][j]*(w[i][k]*ruu[i][j]+v[i][k]*iuu[i][j]-y[i][k]*
                        rtu[i][j]-x[i][k]*itu[i][j])+Im[i][j]*(-v[i][k]*ruu[i][j]+w[i][k]*iuu[i][j]-y
                        [i][k]*itu[i][j]+x[i][k]*rtu[i][j]));
                    abl[2*m*f+f*i+k]+=4*tr[i][j]*(ruu[i][j]*x[j][k]-iuu[i][j]*y[j][k]-rut[i][j]*v[j][k
                        ]+iut[i][j]*w[j][k])-8*(Re[i][j]*(x[j][k]*rtt[i][j]+y[j][k]*itt[i][j]-v[j][k
                        ]*rtu[i][j]-w[j][k]*itu[i][j])+Im[i][j]*(-y[j][k]*rtt[i][j]+x[j][k]*itt[i][j
                        ]+w[j][k]*rtu[i][j]-v[j][k]*itu[i][j]));
                    abl[2*m*f+f*j+k]+=4*tr[i][j]*(ruu[i][j]*x[i][k]+iuu[i][j]*y[i][k]-rtu[i][j]*v[i][k
                        ]-itu[i][j]*w[i][k])-8*(Re[i][j]*(x[i][k]*rtt[i][j]-y[i][k]*itt[i][j]-v[i][k
                        ]*rut[i][j]+w[i][k]*iut[i][j])+Im[i][j]*(y[i][k]*rtt[i][j]+x[i][k]*itt[i][j]-
                        v[i][k]*iut[i][j]-w[i][k]*rut[i][j]));
                    abl[3*m*f+f*i+k]+=4*tr[i][j]*(ruu[i][j]*y[j][k]+iuu[i][j]*x[j][k]-rut[i][j]*w[j][k
                        ]-iut[i][j]*v[j][k])-8*(Re[i][j]*(y[j][k]*rtt[i][j]-x[j][k]*itt[i][j]-w[j][k
                        ]*rtu[i][j]+v[j][k]*itu[i][j])+Im[i][j]*(x[j][k]*rtt[i][j]+y[j][k]*itt[i][j]-
                        v[j][k]*rtu[i][j]-w[j][k]*itu[i][j]));
                    abl[3*m*f+f*j+k]+=4*tr[i][j]*(ruu[i][j]*y[i][k]-iuu[i][j]*x[i][k]-rtu[i][j]*w[i][k
                        ]+itu[i][j]*v[i][k])-8*(Re[i][j]*(y[i][k]*rtt[i][j]+x[i][k]*itt[i][j]-w[i][k
                        ]*rut[i][j]-v[i][k]*iut[i][j])+Im[i][j]*(-x[i][k]*rtt[i][j]+y[i][k]*itt[i][j
                        ]-w[i][k]*iut[i][j]+v[i][k]*rut[i][j]));
                }
            }
        }
}
    for(i=0;i<m;i++)
    {
        for(k=0;k<f;k++)
        {
            abl[f*i+k]+=4*tr[i][i]*(rtt[i][i]*v[i][k]-itt[i][i]*w[i][k]-rtu[i][i]*x[i][k]+itu[i][i]*
                y[i][k])-8*(Re[i][i]*(v[i][k]*ruu[i][i]+w[i][k]*iuu[i][i]-x[i][k]*rut[i][i]-y[i][k
                ]*iut[i][i])+Im[i][i]*(-w[i][k]*ruu[i][i]+v[i][k]*iuu[i][i]+y[i][k]*rut[i][i]-x[i][
                k]*iut[i][i]));
            abl[m*f+f*i+k]+=4*tr[i][i]*(rtt[i][i]*w[i][k]+itt[i][i]*v[i][k]-rtu[i][i]*y[i][k]-itu[i
                ][i]*x[i][k])-8*(Re[i][i]*(w[i][k]*ruu[i][i]-v[i][k]*iuu[i][i]-y[i][k]*rut[i][i]+x[
                i][k]*iut[i][i])+Im[i][i]*(v[i][k]*ruu[i][i]+w[i][k]*iuu[i][i]-x[i][k]*rut[i][i]-y[
                i][k]*iut[i][i]));
            abl[2*m*f+f*i+k]+=4*tr[i][i]*(ruu[i][i]*x[i][k]-iuu[i][i]*y[i][k]-rut[i][i]*v[i][k]+iut[
                i][i]*w[i][k])-8*(Re[i][i]*(x[i][k]*rtt[i][i]+y[i][k]*itt[i][i]-v[i][k]*rtu[i][i]-w
                [i][k]*itu[i][i])+Im[i][i]*(-y[i][k]*rtt[i][i]+x[i][k]*itt[i][i]+w[i][k]*rtu[i][i]-
                v[i][k]*itu[i][i]));
```

```
            abl[3*m*f+f*i+k]+=4*tr[i][i]*(ruu[i][i]*y[i][k]+iuu[i][i]*x[i][k]-rut[i][i]*w[i][k]-iut[
                i][i]*v[i][k])-8*(Re[i][i]*(y[i][k]*rtt[i][i]-x[i][k]*itt[i][i]-w[i][k]*rtu[i][i]+v
                [i][k]*itu[i][i])+Im[i][i]*(x[i][k]*rtt[i][i]+y[i][k]*itt[i][i]-v[i][k]*rtu[i][i]-w
                [i][k]*itu[i][i]));
        }
    }
    if(Z==1) fprintf(fd,"%.20f\t",funk);
    return funk;
}

int restr(double v[][f],double w[][f], double x[][f], double y[][f],double r[][f],double ablr[],
    double lambda[][f], double mu)
{
    int i,j,k,l;
    for(i=0;i<f;i++)
    {
        for(j=0;j<f;j++)  r[i][j]=0;
    }
    for(i=0;i<f;i++)
    {
        for(k=0;k<m;k++) r[i][i]+=x[k][i]*x[k][i]+y[k][i]*y[k][i]-v[k][i]*v[k][i]-w[k][i]*w[k][i];
        r[i][i]--;
    }
    for(i=0;i<f;i++)
    {
        for(j=0;j<i;j++)
        {
            for(k=0;k<m;k++)
            {
                r[i][j]+=x[k][i]*x[k][j]+y[k][i]*y[k][j]-v[k][i]*v[k][j]-w[k][i]*w[k][j];
                r[j][i]+=x[k][i]*y[k][j]-y[k][i]*x[k][j]-v[k][i]*w[k][j]+w[k][i]*v[k][j];
            }
        }
    }
    for(i=0;i<4*m*f;i++) ablr[i]=0;
    for(k=0;k<f;k++)
    {
        for(l=0;l<k;l++)
        {
            for(i=0;i<m;i++)
            {
                ablr[f*i+k]+=-(2*mu*r[k][l]-lambda[k][l])*v[i][l]-(2*mu*r[l][k]-lambda[l][k])*w[i][l
                    ];
                ablr[f*i+l]+=-(2*mu*r[k][l]-lambda[k][l])*v[i][k]+(2*mu*r[l][k]-lambda[l][k])*w[i][k
                    ];
                ablr[m*f+f*i+k]+=-(2*mu*r[k][l]-lambda[k][l])*w[i][l]+(2*mu*r[l][k]-lambda[l][k])*v[i
                    ][l];
                ablr[m*f+f*i+l]+=-(2*mu*r[k][l]-lambda[k][l])*w[i][k]-(2*mu*r[l][k]-lambda[l][k])*v[i
                    ][k];
                ablr[2*m*f+f*i+k]+=(2*mu*r[k][l]-lambda[k][l])*x[i][l]+(2*mu*r[l][k]-lambda[l][k])*y[
                    i][l];
                ablr[2*m*f+f*i+l]+=(2*mu*r[k][l]-lambda[k][l])*x[i][k]-(2*mu*r[l][k]-lambda[l][k])*y[
                    i][k];
                ablr[3*m*f+f*i+k]+=(2*mu*r[k][l]-lambda[k][l])*y[i][l]-(2*mu*r[l][k]-lambda[l][k])*x[
                    i][l];
                ablr[3*m*f+f*i+l]+=(2*mu*r[k][l]-lambda[k][l])*y[i][k]+(2*mu*r[l][k]-lambda[l][k])*x[
                    i][k];
            }
        }
    }
    for(k=0;k<f;k++)
    {
        for(i=0;i<m;i++)
        {
            ablr[f*i+k]+=-2*(2*mu*r[k][k]-lambda[k][k])*v[i][k];
            ablr[m*f+f*i+k]+=-2*(2*mu*r[k][k]-lambda[k][k])*w[i][k];
            ablr[2*m*f+f*i+k]+=2*(2*mu*r[k][k]-lambda[k][k])*x[i][k];
            ablr[3*m*f+f*i+k]+=2*(2*mu*r[k][k]-lambda[k][k])*y[i][k];
        }
    }
    return 0;
}

double cgmin(FILE *fd,  double v[][f], double w[][f], double x[][f], double y[][f], double mu,
    double tau, double lambda[][f])
{
    int i,j,k=1,l;
    double funk,abl[4*m*f],r[f][f],ablr[4*m*f],L=0,p[4*m*f];
    double va[m][f],wa[m][f],xa[m][f],ya[m][f],ra[m][f],La,fa,Labl[4*m*f],Lnorm=0,Lnorm1=0,lp;
    double a=0.1,rs,beta,R;

    funk=func(fd,v,w,x,y,abl,0);
    restr(v,w,x,y,r,ablr,lambda,mu);
    for(i=0;i<f;i++)
    {
        for(j=0;j<f;j++) L=L+mu*r[i][j]*r[i][j]-lambda[i][j]*r[i][j];
    }
    L=funk+L;
    for(i=0;i<4*m*f;i++) Labl[i]=abl[i]+ablr[i];
    Lnorm=0;
    for(i=0;i<4*m*f;i++) Lnorm=Lnorm+Labl[i]*Labl[i];
    for(i=0;i<4*m*f;i++) p[i]=-Labl[i];
```

```
    while(Lnorm>tau && k<100000)
    {
        neu(a,v,w,x,y,va,wa,xa,ya,p);
        fa=func(fd,va,wa,xa,ya,abl,0);
        restr(va,wa,xa,ya,ra,ablr,lambda,mu);
        La=0;
        for(i=0;i<f;i++)
        {
            for(j=0;j<f;j++) La+=mu*ra[i][j]*ra[i][j]-lambda[i][j]*ra[i][j];
        }
        La+=fa;
        lp=0;
        for(i=0;i<4*m*f;i++) lp+=p[i]*Labl[i];
        rs=L+a/1000*lp;
        l=0;
        while(La > rs)
        {
            a=a*2/3;
            neu(a,v,w,x,y,va,wa,xa,ya,p);
            fa=func(fd,va,wa,xa,ya,abl,0);
            restr(va,wa,xa,ya,ra,ablr,lambda,mu);
            La=0;
            for(i=0;i<f;i++)
            {
                for(j=0;j<f;j++) La+=mu*ra[i][j]*ra[i][j]-lambda[i][j]*ra[i][j];
            }
            La+=fa;
            rs=L+a/1000*lp;
            l++;
        }
        for(i=0;i<m;i++)
        {
            for(j=0;j<f;j++)
            {
                v[i][j]=va[i][j];
                w[i][j]=wa[i][j];
                x[i][j]=xa[i][j];
                y[i][j]=ya[i][j];
            }
        }
        funk=func(fd,v,w,x,y,abl,0);
        restr(v,w,x,y,r,ablr,lambda,mu);
        L=0;
        for(i=0;i<f;i++)
        {
            for(j=0;j<f;j++) L+=mu*r[i][j]*r[i][j]-lambda[i][j]*r[i][j];
        }
        L+=funk;
        for(i=0;i<4*m*f;i++) Labl[i]=abl[i]+ablr[i];
        Lnorm1=0;
        for(i=0;i<4*m*f;i++) Lnorm1=Lnorm1+Labl[i]*Labl[i];
        beta=Lnorm1/Lnorm;
        Lnorm=Lnorm1;
        for(i=0;i<4*m*f;i++) p[i]=-Labl[i]+beta*p[i];
        a=0.1;
        k++;
    }
    R=0;
    for(i=0;i<f;i++)
    {
        for(j=0;j<f;j++) R=R+r[i][j]*r[i][j];
    }
    for(i=0;i<f;i++)
    {
        for(j=0;j<f;j++)
        {
            lambda[i][j]=lambda[i][j]-r[i][j]*2*mu;

        }
    }
    return R;
}

int neu(double a, double v[][f], double w[][f], double x[][f], double y[][f], double va[][f],
    double wa[][f], double xa[][f], double ya[][f], double p[])
{
    int i,j;
    for(i=0;i<m;i++)
    {
        for(j=0;j<f;j++)
        {
            va[i][j]=v[i][j]+a*p[f*i+j];
            wa[i][j]=w[i][j]+a*p[m*f+f*i+j];
            xa[i][j]=x[i][j]+a*p[2*m*f+f*i+j];
            ya[i][j]=y[i][j]+a*p[3*m*f+f*i+j];
        }
    }
    return 0;
}
```

Remark: We skipped the comments and the output functions in the code.

# B Solutions of the Variational Principle on Projectors

| f \ m | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0.5 | 0.125 | 0.05556 | 0.03125 | 0.02000 | 0.01389 | 0.01020 | 0.00781 | 0.00617 | 0.00500 |
| 2 | | 1.000 | 0.33333 | 0.16667 | 0.10701 | 0.07407 | 0.05442 | 0.04167 | 0.03292 | 0.02133 |
| 3 | | | 1.50000 | 0.65625 | 0.36712 | 0.22500 | 0.15306 | 0.11198 | 0.08333 | 0.06754 |
| 4 | | | | 2.00000 | 1.04000 | 0.62963 | 0.40816 | 0.28571 | 0.21111 | 0.16003 |
| 5 | | | | | 2.50000 | 1.45833 | 0.94218 | 0.64323 | 0.46421 | 0.34722 |
| 6 | | | | | | 3.00000 | 1.89796 | 1.29167 | 0.91667 | 0.68003 |
| 7 | | | | | | | 3.50000 | 2.35156 | 1.66872 | 1.22756 |
| 8 | | | | | | | | 4.00000 | 2.81481 | 2.06667 |
| 9 | | | | | | | | | 4.50000 | 3.28500 |

Table B.1: The values of $\mathcal{S}_{\min}$

| f \ m | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 1/4 | 1/9 | 1/16 | 1/25 | 1/36 | 1/49 | 1/64 | 1/81 | 1/100 |
| 2 | | 1 | 4/9 | 1/4 | x | 1/9 | 4/49 | 1/16 | 4/81 | x |
| 3 | | | 1 | 9/16 | x | 1/4 | 9/49 | 9/81 | 1/9 | x |
| 4 | | | | 1 | 16/25 | 4/9 | 16/49 | 1/4 | x | x |
| 5 | | | | | 1 | 25/36 | 25/49 | 25/64 | x | 1/4 |
| 6 | | | | | | 1 | 36/49 | 9/16 | 4/9 | x |
| 7 | | | | | | | 1 | 49/64 | 49/81 | x |
| 8 | | | | | | | | 1 | 64/81 | 16/25 |
| 9 | | | | | | | | | 1 | 81/100 |

Table B.2: The according values of $\mathrm{Tr}(A_{xx})$

| f \ m | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | | 1/4 | 1/9 | 1/16 | 1/25 | 1/36 | 1/49 | 1/64 | 1/81 | 1/100 |
| 2 | | 0 | 1/9 | 1/12 | x | x | x | x | x | x |
| 3 | | | 0 | 1/16 | x | 1/20 | 2/49 | x | 1/36 | x |
| 4 | | | | 0 | 1/25 | x | 2/49 | 0.03571 | x | x |
| 5 | | | | | 0 | 1/36 | x | x | x | 1/36 |
| 6 | | | | | | 0 | 1/49 | x | 1/36 | x |
| 7 | | | | | | | 0 | 1/64 | x | x |
| 8 | | | | | | | | 0 | 1/81 | x |
| 9 | | | | | | | | | 0 | 1/100 |

Table B.3: The according values of $\mathrm{Tr}(A_{xy})$ for $x \neq y$

Remark: The placeholder x denotes that the values of the traces do not coincide.

# C Codes used for Global Optimization

Remark: The annealing algorithm contained in the m-file anneal.m is available in [30]. The variable theta is a vector in $\mathbb{R}^{2f}$ and contains the values $\vartheta_i, \varphi_i$ corresponding to the vector $x_i = v(\vartheta_i, \varphi_i)$. We again skip the output functions.

```
function [w,theta]=annealloop(action,tau,thetastart)
% minimizes a function repetitively applying the Simulated annealing algorithm anneal.m
% Input: *action=action(theta,tau) function that calculates the action S on the point theta for
     eigenvalues given by 1 +tau, 1-tau
%         *tau parameter determines the eigenvalues
%         *thetastart starting vector

z=0;k=1;b=0.8;a=0.8;Initmax=100;
wvgl=action(thetastart,tau);
str=struct('InitTemp',max(wvgl,10000),'MaxConsRej',1.0e+3,'StopTemp',1.0e-6,'MaxSuccess',1.0e+3,'
     CoolSched',@(T) (a*T),'MaxTries',100);

wmin=wvgl; thetamin=thetastart;

while str.InitTemp>=Initmax || k<5
    [thetamin2,wmin2]=anneal(@(theta)action(theta,tau),thetamin,str);
    if wmin2<=wmin
        wmin=wmin2;
        thetamin=thetamin2;
        z=0;
    else z=z+1;
    end;
    k=k+1;
    str.InitTemp=str.InitTemp*b;
end;

w=wmin;
theta=thetamin;
```

```
function globmin_sph(action,taumin,h,taumax,m)
% function that finds global minimizer of the function action for different values of tau given
     as taumin, taumin+h, taumin+2h, ..., taumax
% Input: *action=action(theta,tau) function that calculates the action S on the point theta for
     eigenvalues given by 1 +tau, 1-tau
%         *parameters thetamin and thetamax: determine the range of the eigenvalues
%         *stepsize h
theta=load(...); %the points of the Tammes distribution used as starting point
tauvec=[];thetamatrix=[];wvec=[];tau=taumin;

while tau < taumax+h
    [wmin,theta]=annealloop(fwirk,tau,theta);
    tauvec=[tauvec,tau];
    wvec=[wvec,wmin];
    thetamatrix=[thetamatrix;theta];
    tau=tau+h;
end;
```

```
function w=actiontau(theta,tau)
% calculates the action for given vector theta and value tau
N=length(theta);M=N/2;h0=1-2*(1/tau^2);w=0;
for i=1:M
    for j=1:(i-1)
        h=sin(theta(i))*sin(theta(j))*cos(theta(i+M)-theta(j+M))+cos(theta(i))*cos(theta(j));
        if h>=h0
            lagr=1e6*2*tau^2*(2*(1+h)-tau^2*(1-h^2));
        else
            lagr=0;
        end;
        w=w+1/M^2*lagr;
    end;
end;
w=2*w+1e6/M*8*tau^2;
return;
```

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